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NEWS 4 AUG 24 ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS 5 AUG 24 CA/CAPLUS enhanced with legal status information for
U.S. patents
NEWS 6 SEP 09 50 Millionth Unique Chemical Substance Recorded in
CAS REGISTRY
NEWS 7 SEP 11 WPIDS, WPINDEX, and WPIX now include Japanese FTERM
thesaurus
NEWS 8 OCT 21 Derwent World Patents Index Coverage of Indian and
Taiwanese Content Expanded
NEWS 9 OCT 21 Derwent World Patents Index enhanced with human
translated claims for Chinese Applications and
Utility Models
NEWS 10 OCT 27 Free display of legal status information in CA/CAPLUS,
USPATFULL, and USPAT2 in the month of November.

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:29:09 ON 18 NOV 2009

=> file reg

10575147a.trn

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STRUCTURE FILE UPDATES: 16 NOV 2009 HIGHEST RN 1192511-54-8
DICTIONARY FILE UPDATES: 16 NOV 2009 HIGHEST RN 1192511-54-8

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

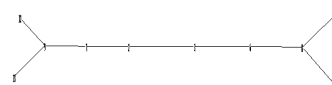
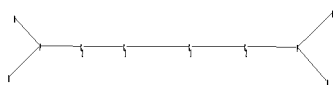
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=>

Uploading C:\Program Files\Stnexp\Queries\10575147\Struc 2.str



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chain nodes :
2 3 6 7 8 9 10 11 12 13
chain bonds :
2-3 2-7 3-6 6-8 7-9 8-10 8-11 9-12 9-13
exact/norm bonds :
2-3 2-7 3-6 6-8 7-9 8-10 8-11 9-12 9-13
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G1:Cb,Cy,Hy

G2:O,S

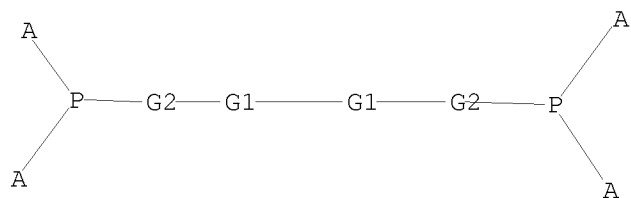
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Match level :
2:CLASS 3:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS
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L1 STRUCTURE UPLOADED

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=> d
L1 HAS NO ANSWERS
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10575147a.trn

L1 STR



G1 Cb,Cy,Hy

G2 O,S

Structure attributes must be viewed using STN Express query preparation.

=> l1

SAMPLE SEARCH INITIATED 09:29:51 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 21817 TO ITERATE

9.2% PROCESSED 2000 ITERATIONS 1 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 427495 TO 445185
 PROJECTED ANSWERS: 20 TO 416

L2 1 SEA SSS SAM L1

=> l1 full

FULL SEARCH INITIATED 09:29:54 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 436995 TO ITERATE

100.0% PROCESSED 436995 ITERATIONS (2 INCOMPLETE) 518 ANSWERS
 SEARCH TIME: 00.00.13

L3 518 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	185.88	186.10

FILE 'CAPLUS' ENTERED AT 09:30:16 ON 18 NOV 2009
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FILE COVERS 1907 - 18 Nov 2009 VOL 151 ISS 21
FILE LAST UPDATED: 17 Nov 2009 (20091117/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

During November, try the new LSUS format of legal status information in the CA/CAPLUS family databases for free! Complete details on the number of free displays and other databases participating in this offer appear in NEWS 10.

=> 13

L4 410 L3

=> 14 monodentate

MISSING OPERATOR L4 MONODENTATE

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> 14 and monodentate

10264 MONODENTATE

L5 9 L4 AND MONODENTATE

=> d ibib abs hitstr 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2009:1259483 CAPLUS

DOCUMENT NUMBER: 151:484111

TITLE: Storage of transition metal complex catalysts bearing polydentate ligands having P-O bonds, and isomerization of allyl compounds with the stored catalysts

INVENTOR(S): Izawa, Yusuke; Utsunomiya, Masaru; Sanba, Yasuhiko; Okubo, Miwako

PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 26pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

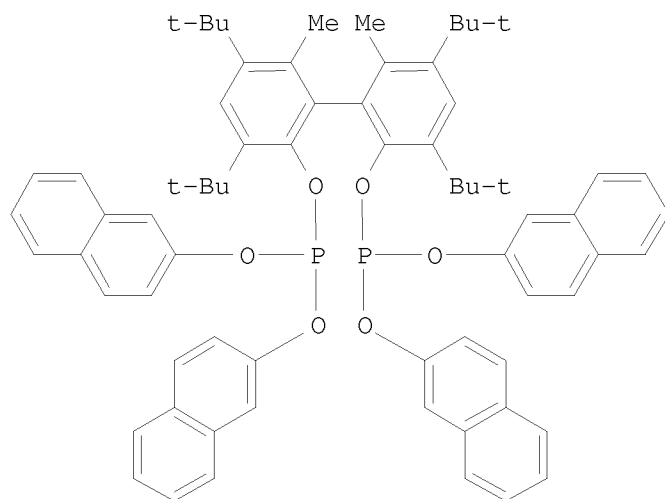
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2009233659	A	20091015	JP 2009-46757	20090227
PRIORITY APPLN. INFO.:			JP 2008-54899	A 20080305
GI				



I

AB The transition metal complex catalysts are stored in the presence of monodentate phosphines and/or polydentate aryl phosphines as antioxidants. Thus, Pd(OAc)₂ was treated with bidentate phosphite ligand I in the presence of PPh₃ in PhMe at 80° for 1 h to give a catalyst solution, which was stored at 80° for 24 h. 3,4-Diacetoxy-1-butene (II) was isomerized in the presence of the stored catalyst solution and AcOH at 130° for 3 h to give a 32:68 mixture of 1,4-diacetoxy-2-butene/II.

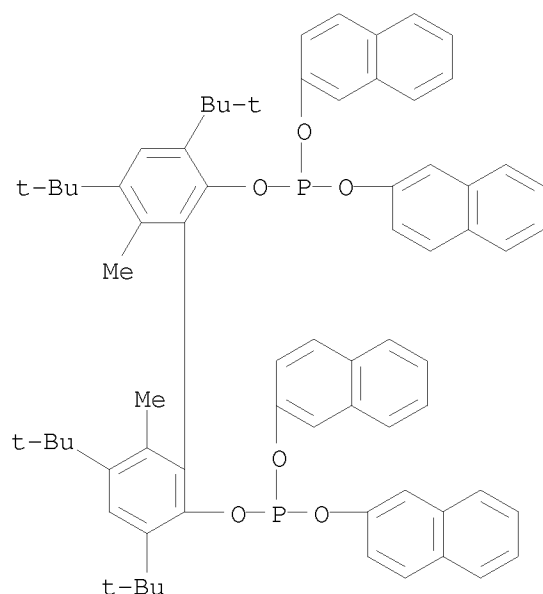
IT 403484-12-8P

RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)

(storage of transition metal complex catalysts bearing polydentate ligands having P-O bonds by using monodentate phosphines and/or polydentate aryl phosphines as antioxidants)

RN 403484-12-8 CAPLUS

CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-2-naphthalenyl ester (CA INDEX NAME)



L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:315029 CAPLUS

DOCUMENT NUMBER: 148:472113

TITLE: Computational descriptors for chelating P,P- and P,N-donor ligands

AUTHOR(S): Fey, Natalie; Harvey, Jeremy N.; Lloyd-Jones, Guy C.; Murray, Paul; Orpen, A. Guy; Osborne, Robert; Purdie, Mark

CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

SOURCE: Organometallics (2008), 27(7), 1372-1383

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ligand knowledge base approach (LKB) has been extended to capture the properties of 108 bidentate P,P- and P,N-donor ligands (1, L1L2). Several parameters, bite angle for square-planar palladium and tetrahedral zinc chelates $\text{cis}[(\text{L1L2})\text{PdCl}_2]$ (2), $[(\text{L1L2})\text{ZnCl}_2]$ (3), L-M and M-Cl bond lengths (M = Pd, Zn), dissociation free energies for 3, steric requirements evaluated as energy of L1L2-He8-hedge association energy were computed at DFT and MM level for the 108 bidentate ligands L1L2. Frontier orbital energies (EHOMO, ELUMO) and proton affinities (PA) were estimated for ligands 1 by calcn. of these values for truncated monodentate versions. The ligands set 1 is therewith described by a range of DFT-calculated descriptors, capturing ligand properties in a variety of chemical environments. New challenges arising from ligand conformational flexibility and donor asymmetry are discussed, and descriptors are related to other parameters, such as the ligand bite angle. A novel map of bidentate ligand space, potentially useful in catalyst design and discovery, has been derived from principal component anal. of the resulting descriptors. In addition, a range of multiple linear regression

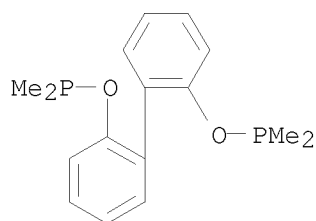
models were derived for both exptl. and calculated data, considering ligand bite angles in square-planar palladium complexes and ligand dissociation energies from octahedral chromium complexes, resp. These data sets were fitted with models based on LKB descriptors to explore the transferability of descriptors to different coordination environments and to illustrate potential applications of such models in catalyst design, allowing predictions about novel or untested ligands.

IT 1018429-17-8 1018429-47-4

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(binding energy, bite angle bond lengths, steric and electronic properties for bidentate diphosphine and phosphine-amine ligands and their metal complexes)

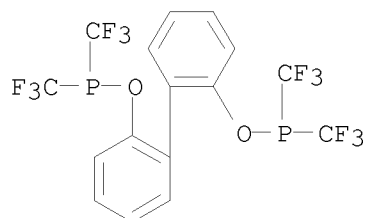
RN 1018429-17-8 CAPLUS

CN Phosphinous acid, P,P-dimethyl-, P,P'-[1,1'-biphenyl]-2,2'-diyl ester (CA INDEX NAME)



RN 1018429-47-4 CAPLUS

CN Phosphinous acid, P,P-bis(trifluoromethyl)-, P,P'-[1,1'-biphenyl]-2,2'-diyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)
REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:992727 CAPLUS

DOCUMENT NUMBER: 141:425573

TITLE: Process for production of dinitriles by butadiene hydrocyanation

INVENTOR(S): Bourgeois, Damien; Rosier, Cecile; Leconte, Philippe

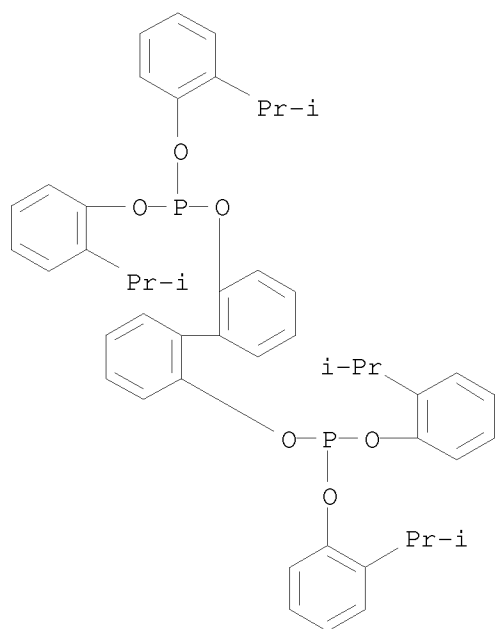
PATENT ASSIGNEE(S): Rhodia Polyamide Intermediates, Fr.

SOURCE: Fr. Demande, 18 pp.

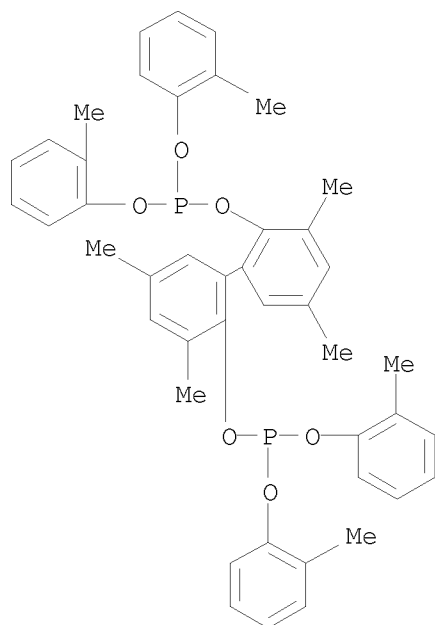
CODEN: FRXXBL

DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2854892	A1	20041119	FR 2003-5673	20030512
FR 2854892	B1	20050624		
WO 2004101498	A2	20041125	WO 2004-FR1110	20040507
WO 2004101498	A3	20050127		
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1622863	A2	20060208	EP 2004-742669	20040507
EP 1622863	B1	20080813		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1787991	A	20060614	CN 2004-80012864	20040507
CN 100441566	C	20081210		
JP 2007502854	T	20070215	JP 2006-530334	20040507
RU 2299194	C2	20070520	RU 2005-138494	20040507
AT 404530	T	20080815	AT 2004-742669	20040507
KR 2006040585	A	20060510	KR 2005-721384	20051110
IN 2005CN02976	A	20070727	IN 2005-CN2976	20051111
US 20070155979	A1	20070705	US 2006-556628	20060921
US 7612223	B2	20091103		
PRIORITY APPLN. INFO.:				
			FR 2003-5673	A 20030512
			WO 2004-FR1110	W 20040507
AB The process comprises at least a stage of butadiene hydrocyanation in the presence of a catalytic system containing an organometallic complex having ≥ 1 monodentate organophosphite ligand and ≥ 1 bidentate organophosphorus ligand and optional promoter such as Lewis acid, a stage of distillation to sep. and recover the catalyst. The distillation is done at a molar ratio of organo-P ligand (as P atom) to the number of metal atom of ≤ 15 , or/and at the weight concentration of metal element of $\leq 1.3\%$ and a bottom temperature of $\leq 180^\circ$.				
IT 178941-51-0D, metal complex 220472-84-4D, metal complex 330976-81-3D, metal complex				
RL: CAT (Catalyst use); USES (Uses) (catalyst recovery in process for production of dinitriles by butadiene hydrocyanation)				
RN 178941-51-0 CAPLUS				
CN Phosphorous acid, [1,1'-biphenyl]-2,2'-diyl tetrakis[2-(1-methylethyl)phenyl] ester (9CI) (CA INDEX NAME)				

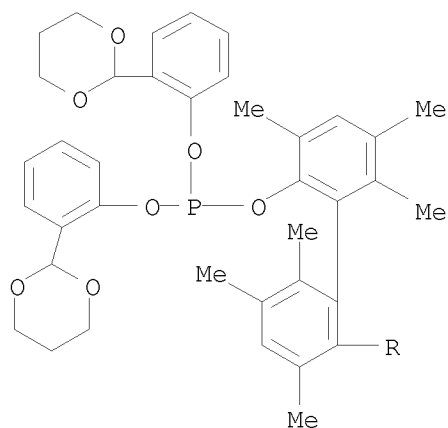


RN 220472-84-4 CAPLUS
 CN Phosphorous acid, P,P'-(3,3',5,5'-tetramethyl[1,1'-biphenyl]-2,2'-diyl)
 P,P,P',P'-tetrakis(2-methylphenyl) ester (CA INDEX NAME)

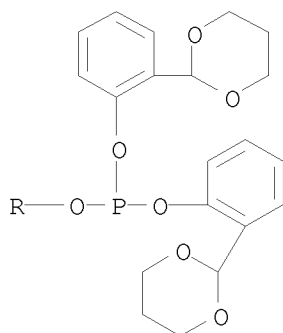


RN 330976-81-3 CAPLUS
 CN Phosphorous acid, 3,3',5,5',6,6'-hexamethyl[1,1'-biphenyl]-2,2'-diyl
 tetrakis[2-(1,3-dioxan-2-yl)phenyl] ester (9CI) (CA INDEX NAME)

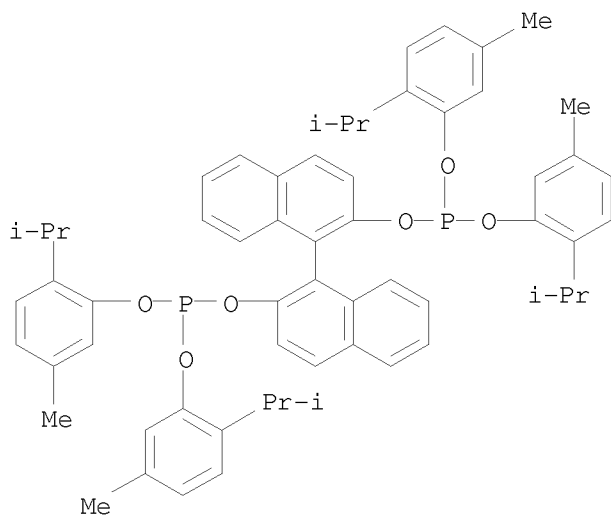
PAGE 1-A



PAGE 2-A



IT 178941-67-8D, metal complex
 RL: CAT (Catalyst use); USES (Uses)
 (hydrocyanation catalyst; catalyst recovery in process for production of
 dinitriles by butadiene hydrocyanation)
 RN 178941-67-8 CAPLUS
 CN Phosphorous acid, [1,1'-binaphthalene]-2,2'-diyl
 tetrakis[5-methyl-2-(1-methylethyl)phenyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:756724 CAPLUS

DOCUMENT NUMBER: 141:260889

TITLE: Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions

INVENTOR(S): Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078766	A1	20040916	WO 2003-US5790	20030227
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003219901	A1	20040928	AU 2003-219901	20030227
WO 2004076464	A2	20040910	WO 2004-US3367	20040227
WO 2004076464	A3	20041216		

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 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

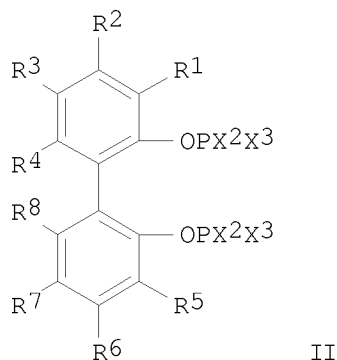
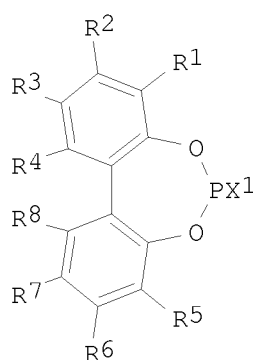
WO 2003-US5790

A 20030227

OTHER SOURCE(S):

MARPAT 141:260889

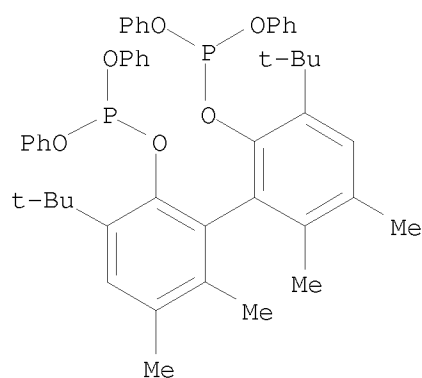
GI



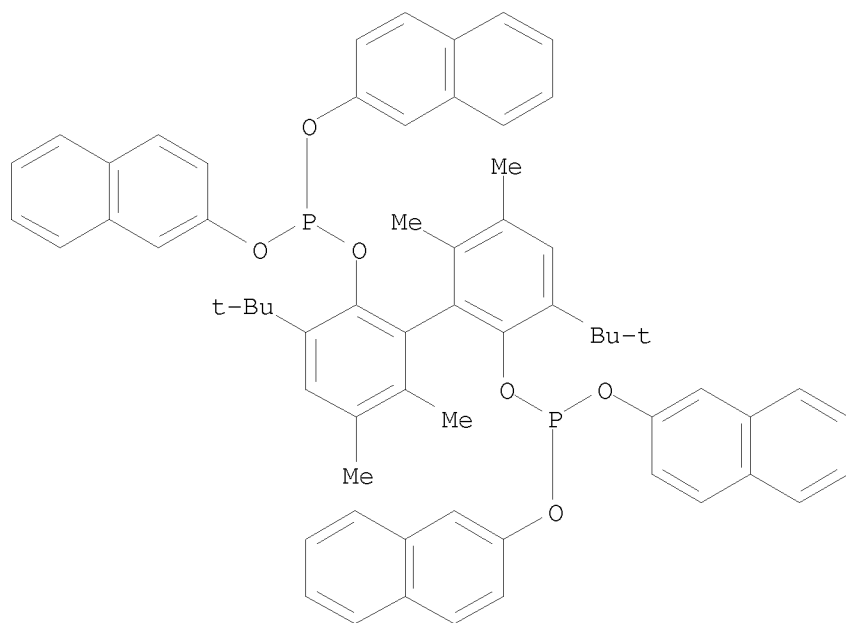
AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 = (NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic

acid with 70.1% ee; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = OPh, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et₂Zn to 2-cyclohexenone affording (S)-3-methylcyclohexanone with 35% ee.

IT 753016-20-5P 753016-21-6P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)
 (asym. ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
 RN 753016-20-5 CAPLUS
 CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetraphenyl ester (9CI) (CA INDEX NAME)



RN 753016-21-6 CAPLUS
 CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



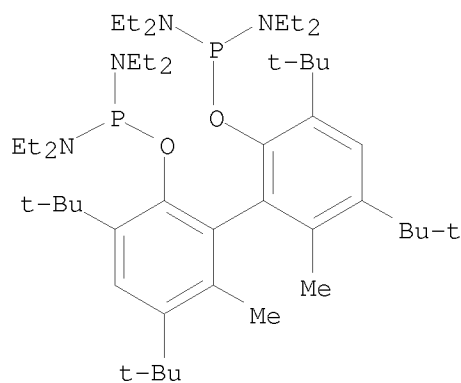
IT 753016-24-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deamination; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-24-9 CAPLUS

CN Phosphorodiamidous acid, tetraethyl-,
(1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



IT 753016-25-0P, [(S)-3,3',5,5'-Tetra-tert-butyl-6,6'-dimethyl-1,1'-biphenyl-2,2'-diyl] bis(phosphorodichloridite)

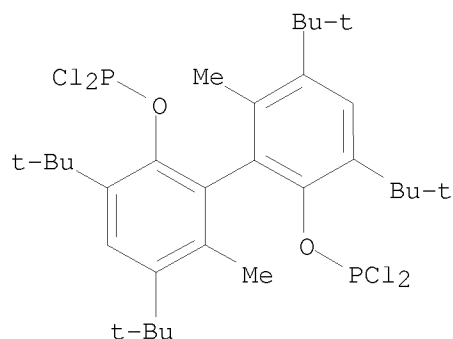
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(esterification; preparation of axially chiral nonracemic mono- and

diphosphite and phosphoramidite ligands for asym. hydrogenation,
hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-25-0 CAPLUS

CN Phosphorodichloridous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-
6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



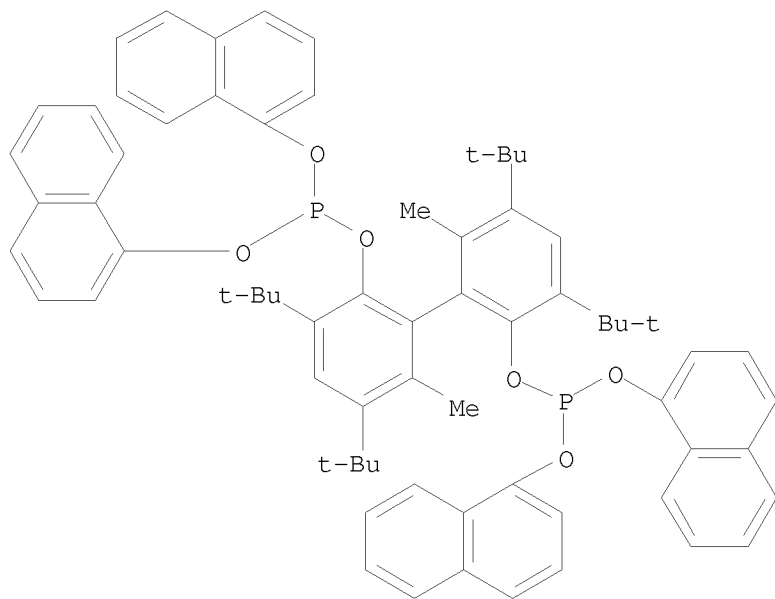
IT 753016-22-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of axially chiral nonracemic mono- and diphosphite and
phosphoramidite ligands for asym. hydrogenation, hydroformylation,
Michael addition and allylic alkylation catalysts)

RN 753016-22-7 CAPLUS

CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-
dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-1-naphthalenyl ester (9CI) (CA
INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:740336 CAPLUS

DOCUMENT NUMBER: 141:243687

TITLE: Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions

INVENTOR(S): Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi; Urata, Hisao

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

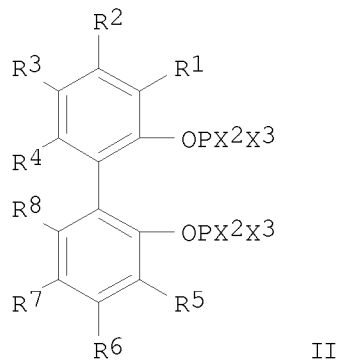
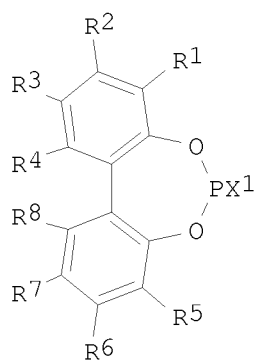
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004076464	A2	20040910	WO 2004-US3367	20040227
WO 2004076464	A3	20041216		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2004078766	A1	20040916	WO 2003-US5790	20030227
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: WO 2003-US5790 A 20030227

OTHER SOURCE(S): MARPAT 141:243687

GI



AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 = (NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic acid with 70.1% ee; (S)-3-methyl-4-oxobutanenitrile was obtained with 96% regioselectivity and 80% ee by asym hydroformylation of 3-butenenitrile; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = N[(R)-CHMePh]2, R1 = R3 = R4 = R5 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et2Zn to 2-cycloheptenone affording (S)-3-methylcycloheptanone with 97.5% ee.

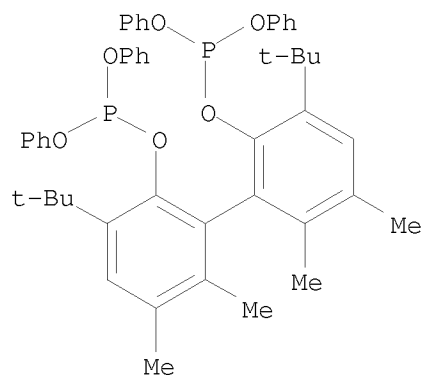
IT 753016-20-5P 753016-21-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(asym. addition ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

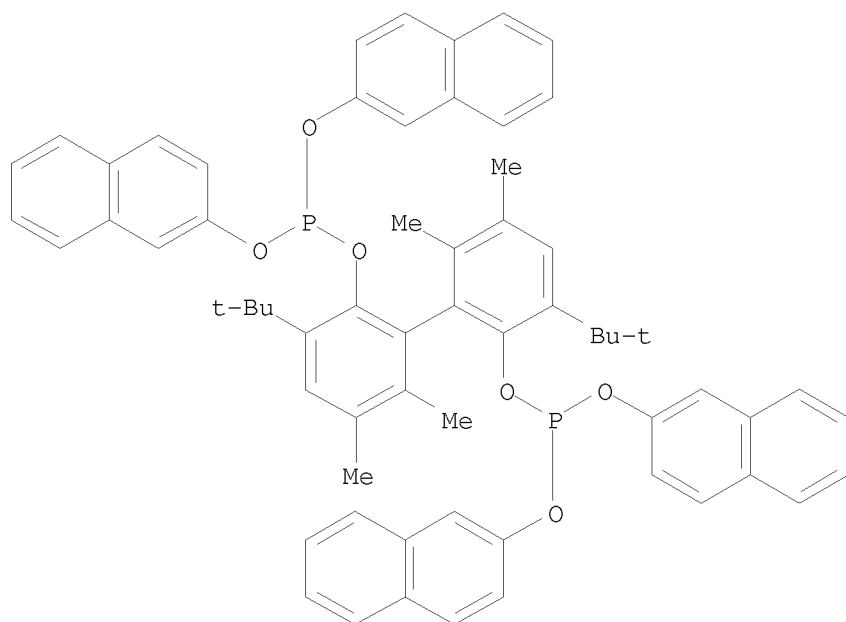
RN 753016-20-5 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetraphenyl ester (9CI) (CA INDEX NAME)



RN 753016-21-6 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

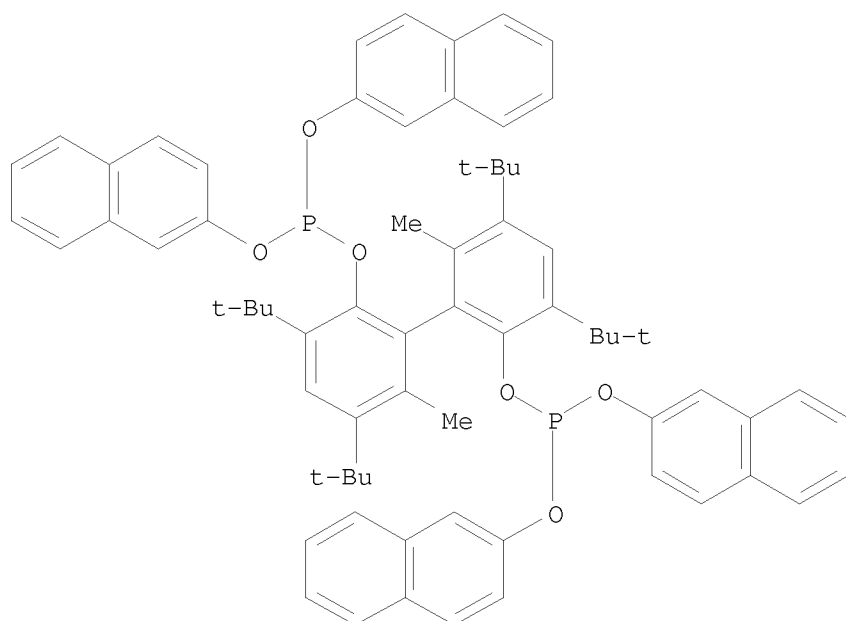


IT 753016-30-7P 753016-35-2P

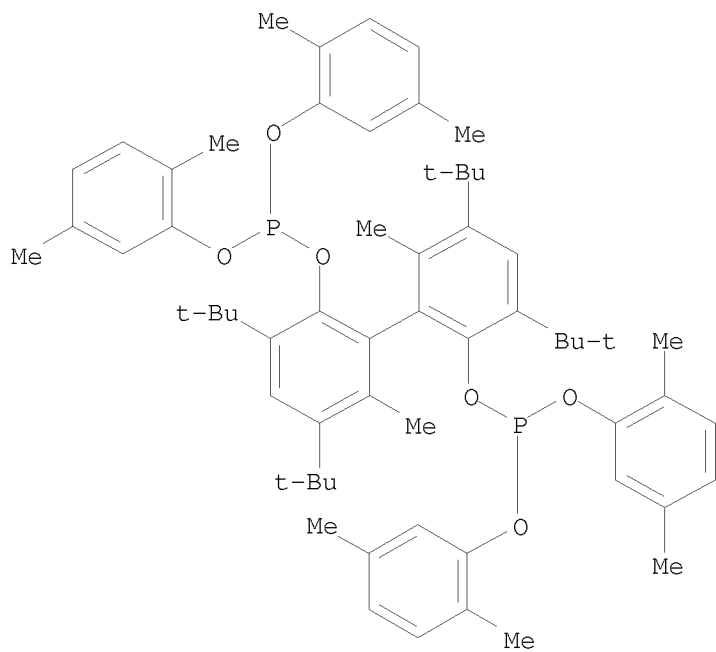
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(asym. hydrogenation ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

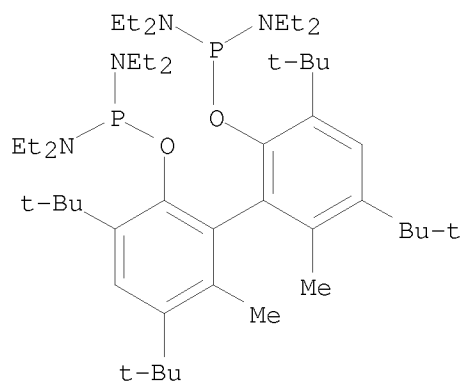
RN 753016-30-7 CAPLUS
 CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-
 dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA
 INDEX NAME)



RN 753016-35-2 CAPLUS
 CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-
 dimethyl[1,1'-biphenyl]-2,2'-diyl tetrakis(2,6-dimethylphenyl) ester (9CI)
 (CA INDEX NAME)



IT 753016-24-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (deamination; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
 RN 753016-24-9 CAPLUS
 CN Phosphorodiamidous acid, tetraethyl-,
 (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)

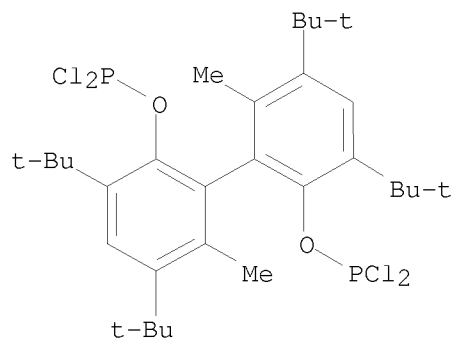


IT 753016-25-0P, [(S)-3,3',5,5'-Tetra-tert-butyl-6,6'-dimethyl-1,1'-biphenyl-2,2'-diyl] bis(phosphorodichloridite)
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(esterification; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-25-0 CAPLUS

CN Phosphorodichloridous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



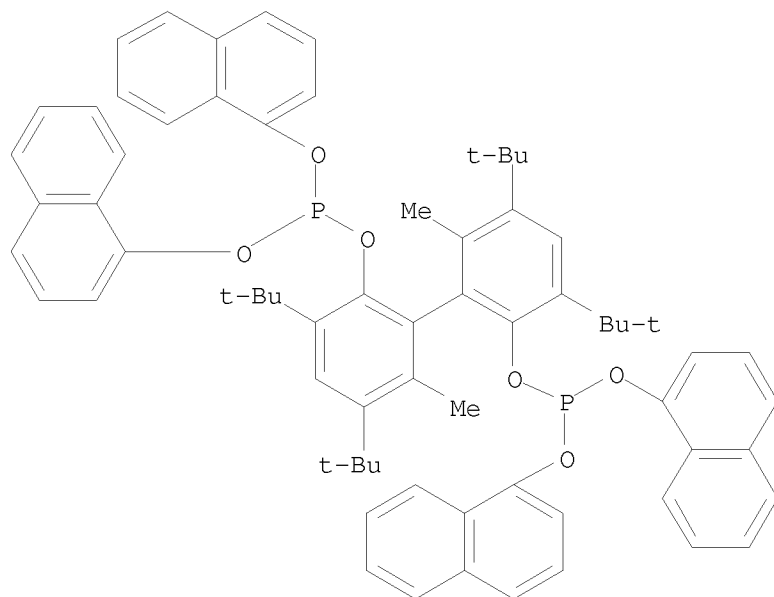
IT 753016-22-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-22-7 CAPLUS

CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-1-naphthalenyl ester (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

(2 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:354301 CAPLUS
DOCUMENT NUMBER: 140:356943
TITLE: Preparation of allyl compounds
INVENTOR(S): Tanaka, Yoshiyuki; Takai, Masaki
PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 56 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004131491	A	20040430	JP 2003-315716	20030908
US 20040147757	A1	20040729	US 2003-648210	20030827
US 7119222	B2	20061010		
US 20050075518	A1	20050407	US 2003-650697	20030829
US 7173157	B2	20070206		
US 20060106181	A1	20060518	US 2005-300290	20051215
US 7241857	B2	20070710		
PRIORITY APPLN. INFO.:			JP 2002-261870	A 20020906
			JP 2002-252900	A 20020830
			JP 2002-252901	A 20020830
			JP 2002-260452	A 20020905
			US 2003-648210	A3 20030827

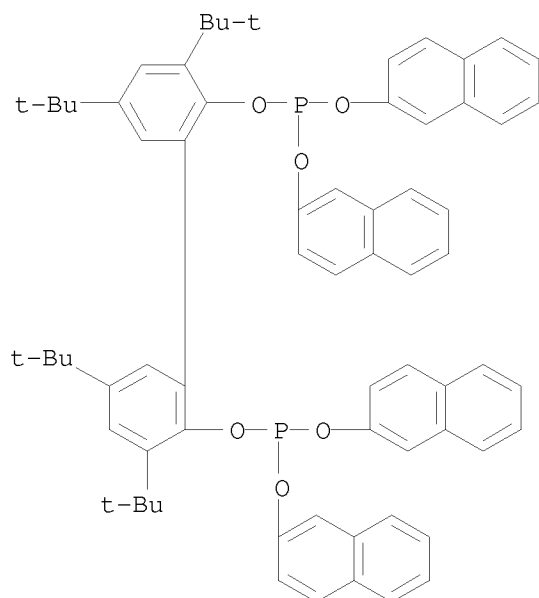
OTHER SOURCE(S): MARPAT 140:356943

AB Allyl compds. are prepared by reaction of allyl compound reactants with nucleophiles by using catalysts containing transition metal compds. having ≥ 1 Group 8-10 transition metals and monodentate ligands P(OR1)(OR2)(OR3) [R1-R3 = (un)substituted alkyl] in the presence of ammonium compds. in the reaction system. Multidentate ligands of phosphites can be also used as catalysts. AcOH was treated with 3,4-diacetoxy-1-butene in the presence of 4-methoxypyridine and a catalyst prepared from trisdibenzylideneacetonedipalladium and tetra(1-naphthyl) 3,3',-5,5'-tetra-(tert-butyl)-6,6'-dimethyl-1'1'-biphenyl-2'2'-diyl diphosphite at 120° to give 1,4-diacetoxy-2-butene [198979-98-5] with reaction rate constant 0.88 h⁻¹.

IT 198979-95-2 198979-98-5 403484-12-8
RL: CAT (Catalyst use); USES (Uses)
(catalyst ligand; preparation of allyl compds. by reaction of allyl compound reactants with nucleophiles in the presence of ammonium compds. and transition metal catalysts)

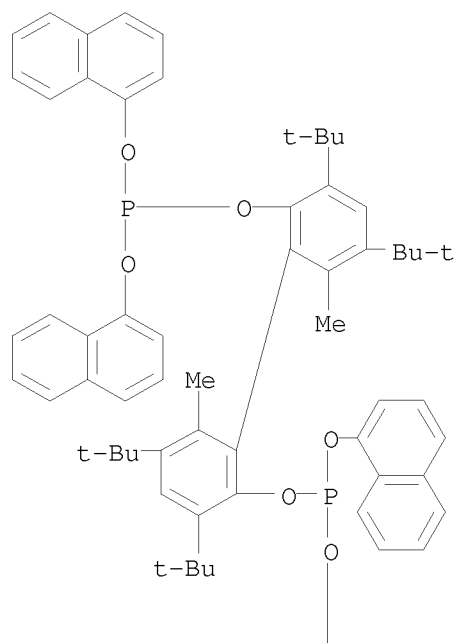
RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

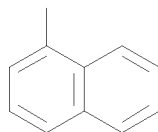


RN 198979-98-5 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-1-naphthalenyl ester (CA INDEX NAME)

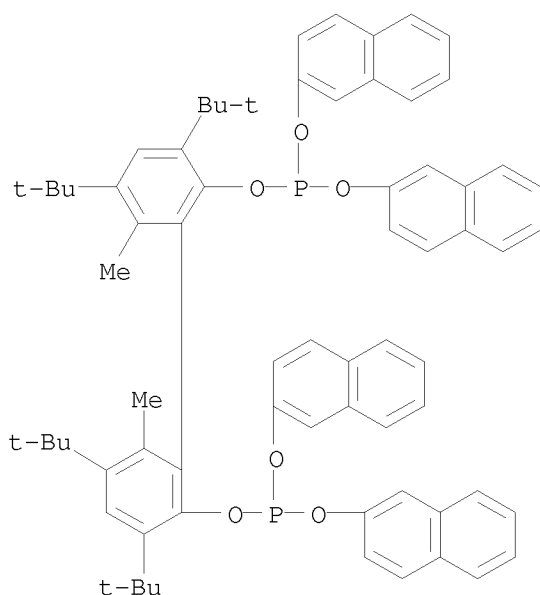
PAGE 1-A



PAGE 2-A



RN 403484-12-8 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-2-naphthalenyl ester
 (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
 (1 CITINGS)

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:596871 CAPLUS

DOCUMENT NUMBER: 131:228491

TITLE: Method of preparation of aldehyde by selective
 hydroformylation of olefin in presence of monovalent
 phosphite compound

INVENTOR(S): Wada, Yasuhiro; Tanaka, Yoshiyuki; Urata, Takao

PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan

SOURCE: Jpn. Kokai Tokyo Koho, 27 pp.

CODEN: JKXXAF

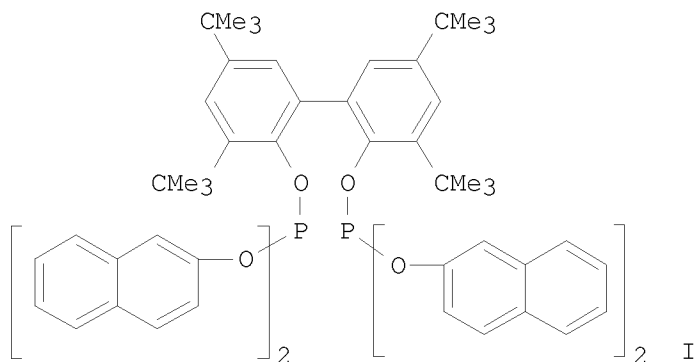
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 11255696	A	19990921	JP 1998-56503	19980309
JP 3903575	B2	20070411		
PRIORITY APPLN. INFO.:			JP 1998-56503	19980309
OTHER SOURCE(S):		CASREACT 131:228491; MARPAT 131:228491		
GI				



AB In preparation of an aldehyde by hydroformylation of olefin with carbon monoxide and hydrogen in the presence of a group VIII metal and an organic polydentate phosphite, the reaction is carried out in the presence of a monodentate phosphite represented by formula $\text{Ar}_3\text{-P}(\text{OAr}_1)\text{OAr}_2$ [Ar_1 - Ar_3 = (un)substituted aromatic organic group, provided that at least two of Ar_1 - Ar_3 possess a branched hydrocarbonyl group at one of the two positions ortho to the phosphite oxygen atom and hydrogen at the other position] in the reaction system. The copresence of the monodentate phosphite ligand improves the catalyst activity and selectivity in a continuous operation and suppresses the side reaction, i.e. reduction of olefins, and can stably provide straight-chain aldehydes which are industrially useful. Thus, 55 mL PhMe, 5 mL heptane, 19.7 mg $[\text{Rh}(\text{OAc})(\text{COD})]_2$ (COD = 1,5-cyclooctadiene), divalent phosphite (I) 2.0 mol/1 g atom Rh, and tris[3,6,8-tri(tert-butyl)-2-naphthyl] phosphite (monovalent phosphite) 4.0 mol/1 g atom Rh were charged in an autoclave. After closing the autoclave and thoroughly purging the inside of the autoclave with N₂, 4.50 g propylene was introduced under pressure followed by introducing water gas (CO/H₂) to a total pressure of 10.0 atm, and the reaction mixture was allowed to react for 1.03-2.60 h while keeping the pressure constant by feeding water gas through a automated pressure regulator to give n-butanal with 97.6% selectivity.

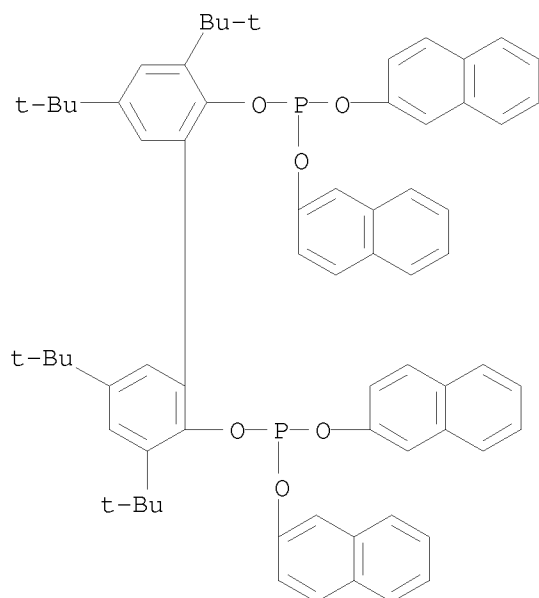
IT 198979-95-2 198979-98-5

RL: CAT (Catalyst use); USES (Uses)

(preparation of aldehyde by selective hydroformylation of olefin with carbon monoxide and hydrogen in presence of group VIII metal-bidentate phosphite complex and monodentate phosphite)

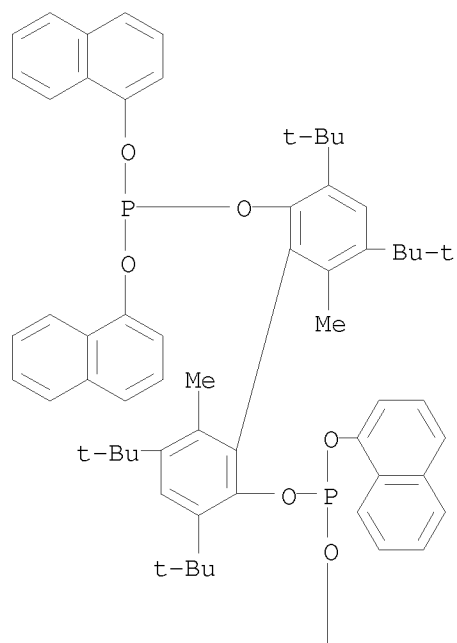
RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

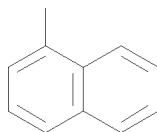


RN 198979-98-5 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-1-naphthalenyl ester (CA INDEX NAME)

PAGE 1-A



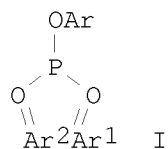
PAGE 2-A



L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1999:583153 CAPLUS
 DOCUMENT NUMBER: 131:199415
 TITLE: Preparation of aldehydes
 INVENTOR(S): Wada, Yasuhiro; Tanaka, Yoshiyuki; Urata, Takao
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11246464	A	19990914	JP 1998-52999	19980305
PRIORITY APPLN. INFO.:			JP 1998-52999	19980305
OTHER SOURCE(S):		MARPAT 131:199415		

GI



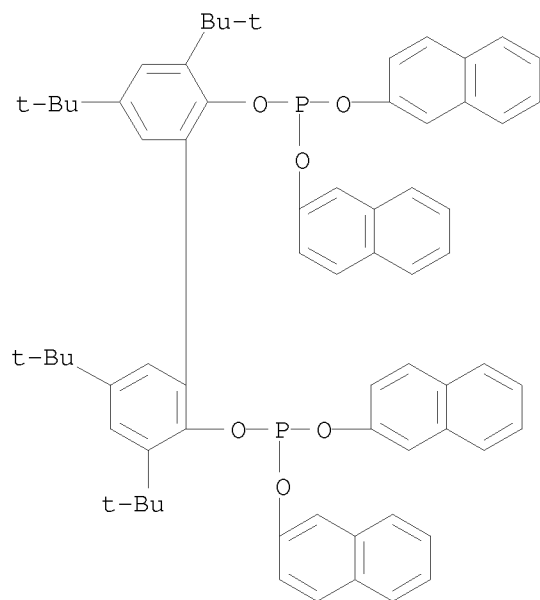
AB Title compds. are prepared by hydroformylation of olefins with CO and H in the presence of cyclic monodentate phosphites I (Ar1, Ar2 = ≥ 1 branched hydrocarbyl-substituted divalent aromatic organic group; Ar = aromatic organic group having no bulky group at o-position to OP) and catalysts containing Group VIII metals and organic multidentate phosphites. Propylene was reacted with a H₂/CO gaseous mixture in the presence of Rh[(OAc)(COD)]₂, Q1[OPQ22]₂ (Q1 = 2,4-tert-butyl-1,6-phenylene-3,5-tert-butyl-1,6-phenylene, Q2 = 2-naphthyl), and I (Ar1Ar2 = same as Q1, Ar = 2-naphthyl) in PhMe at 70° under 10.0 atm for 0.85-1.10 h to give n-aldehyde with 97.9% selectivity.

IT 198979-95-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalyst ligand; preparation of aldehydes by hydroformylation of olefins with Group VIII metal-multidentate phosphite catalysts and cyclic

monodentate phosphites)

RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



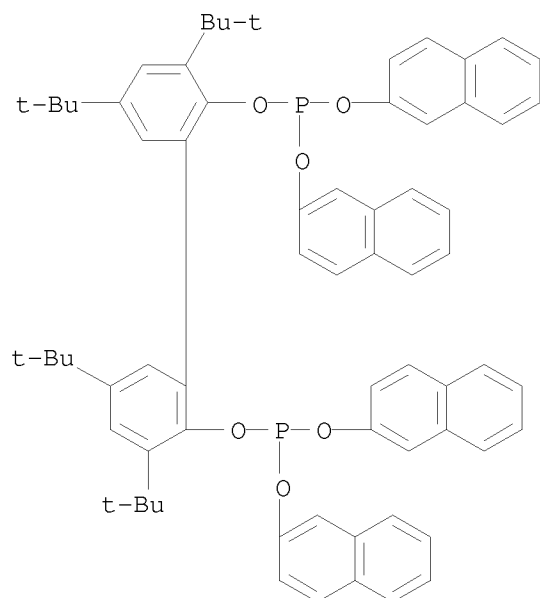
IT 198979-95-2D, complex with Rh

RL: CAT (Catalyst use); USES (Uses)

(preparation of aldehydes by hydroformylation of olefins with Group VIII metal-multidentate phosphite catalysts and cyclic monodentate phosphites)

RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:300852 CAPLUS

DOCUMENT NUMBER: 128:323141

ORIGINAL REFERENCE NO.: 128:64031a,64034a

TITLE: Process for preparation of an aldehyde by hydroformylation of an unsaturated organic compound

INVENTOR(S): Borman, Peter Cornelis; Gelling, Onko Jan

PATENT ASSIGNEE(S): DSM N.V., Neth.

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 839787	A1	19980506	EP 1996-203070	19961104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2270521	A1	19980514	CA 1997-2270521	19971030
WO 9819984	A1	19980514	WO 1997-NL595	19971030
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9858830	A	19980529	AU 1998-58830	19971030
EP 937023	A1	19990825	EP 1997-954493	19971030
EP 937023	B1	20011004		

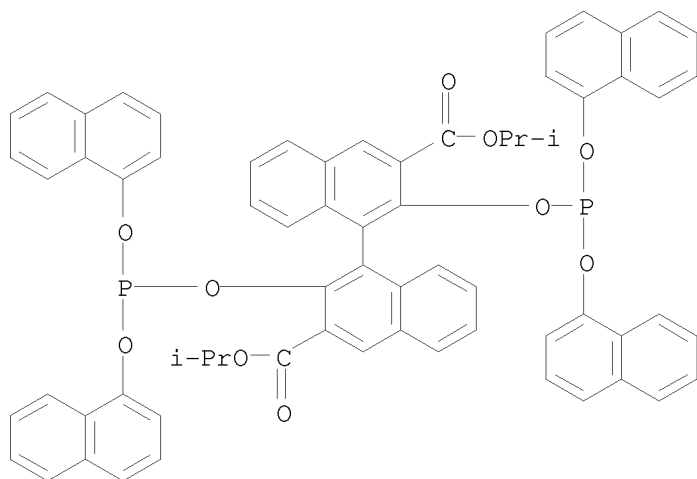
EP 937023	B2	20060208		
R: BE, DE, ES, FR, GB, IT, NL				
CN 1241993	A	20000119	CN 1997-181069	19971030
CN 1117723	C	20030813		
JP 2001504099	T	20010327	JP 1998-521246	19971030
ES 2165102	T3	20020301	ES 1997-954493	19971030
US 6153800	A	20001128	US 1999-303680	19990503
KR 2000053058	A	20000825	KR 1999-703967	19990504
HK 1024465	A1	20040507	HK 2000-103790	20000622
PRIORITY APPLN. INFO.:			EP 1996-203070	A 19961104
			US 1996-32672P	P 19961209
			WO 1997-NL595	W 19971030

OTHER SOURCE(S): MARPAT 128:323141

AB The process uses a catalyst system comprising rhodium or iridium, a multidentate organic phosphite ligand, and a monodentate phosphine. The process can advantageously be carried out for the preparation of Me 5-formylvalerate, which is an intermediate in the preparation of ϵ -caprolactam or adipic acid, which are in turn raw materials for the preparation of nylon 6 and nylon 66, resp.

IT 196299-56-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts for preparation of aldehydes by hydroformylation of unsatd. organic compds.)

RN 196299-56-6 CAPLUS
 CN [1,1'-Binaphthalene]-3,3'-dicarboxylic acid, 2,2'-bis[[bis(1-naphthalenyloxy)phosphino]oxy]-, 3,3'-bis(1-methylethyl) ester (CA INDEX NAME)



OS.CITING REF COUNT:	4	THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT:	4	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 COST IN U.S. DOLLARS

SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	54.00	240.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.38	-7.38

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PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 09:36:12 ON 18 NOV 2009
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	54.00	240.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.38	-7.38

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	54.00	240.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.38	-7.38

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STRUCTURE FILE UPDATES: 16 NOV 2009 HIGHEST RN 1192511-54-8
DICTIONARY FILE UPDATES: 16 NOV 2009 HIGHEST RN 1192511-54-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

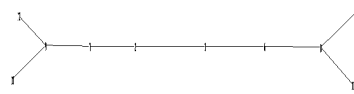
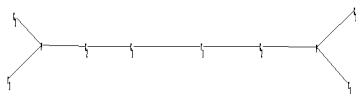
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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Uploading C:\Program Files\Stnexp\Queries\10575147\Struc 3.str



chain nodes :
2 3 6 7 8 9 10 11 12 13
chain bonds :
2-3 2-7 3-6 6-8 7-9 8-10 8-11 9-12 9-13
exact/norm bonds :
2-3 2-7 3-6 6-8 7-9 8-10 8-11 9-12 9-13

G1:Cb,Cy,Hy

G2:O,S

G3:A,Cb,Cy,Hy

Match level :

10575147a.trn

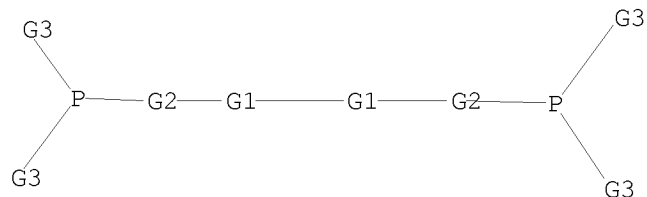
2:CLASS 3:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
13:CLASS

L6 STRUCTURE UPLOADED

=> d

L6 HAS NO ANSWERS

L6 STR



G1 Cb,Cy,Hy

G2 O,S

G3 A,Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> 16

SAMPLE SEARCH INITIATED 09:36:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 21845 TO ITERATE

9.2% PROCESSED 2000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 428050 TO 445750
PROJECTED ANSWERS: 156 TO 716

L7 2 SEA SSS SAM L6

=> 16 full

FULL SEARCH INITIATED 09:36:37 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 437426 TO ITERATE

100.0% PROCESSED 437426 ITERATIONS (2 INCOMPLETE) 741 ANSWERS
SEARCH TIME: 00.00.09

L8 741 SEA SSS FUL L6

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	425.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.38

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FILE COVERS 1907 - 18 Nov 2009 VOL 151 ISS 21
 FILE LAST UPDATED: 17 Nov 2009 (20091117/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

During November, try the new LSUS format of legal status information in the CA/CAPLUS family databases for free! Complete details on the number of free displays and other databases participating in this offer appear in NEWS 10.

=> 18

L9 505 L8

=> 19 and monodentate

10264 MONODENTATE

L10 13 L9 AND MONODENTATE

=> 19 not 15

L11 496 L9 NOT L5

=> 110 not 15

L12 4 L10 NOT L5

=> d ibib abs hitstr 110 1-13

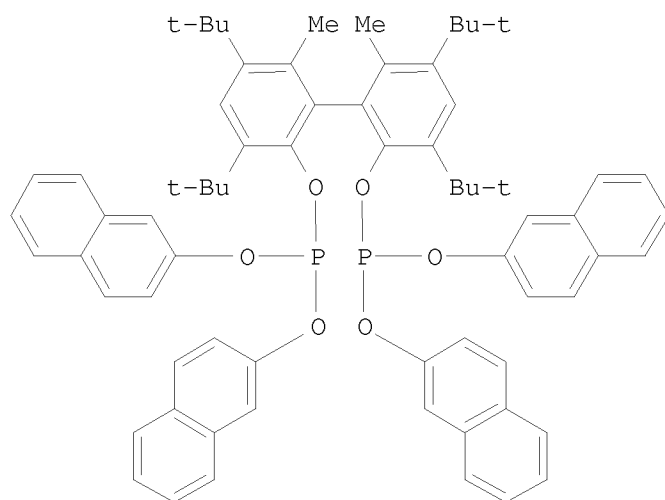
L10 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2009:1259483 CAPLUS

10575147a.trn

DOCUMENT NUMBER: 151:484111
 TITLE: Storage of transition metal complex catalysts bearing polydentate ligands having P-O bonds, and isomerization of allyl compounds with the stored catalysts
 INVENTOR(S): Izawa, Yusuke; Utsunomiya, Masaru; Sanba, Yasuhiko; Okubo, Miwako
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 26pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2009233659	A	20091015	JP 2009-46757	20090227
PRIORITY APPLN. INFO.:			JP 2008-54899	A 20080305

GI

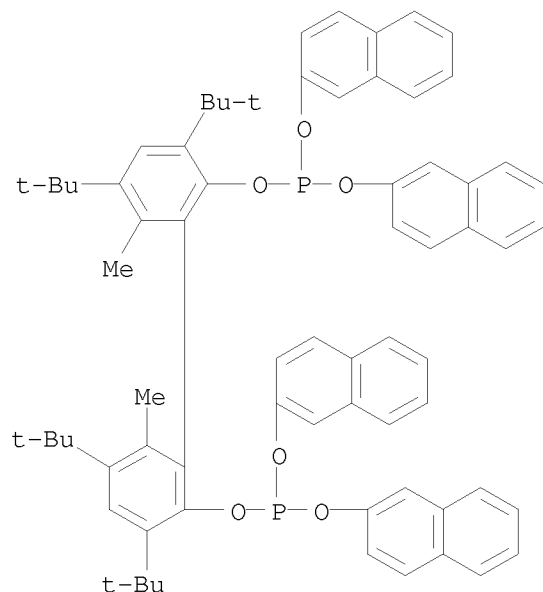


AB The transition metal complex catalysts are stored in the presence of monodentate phosphines and/or polydentate aryl phosphines as antioxidants. Thus, Pd(OAc)₂ was treated with bidentate phosphite ligand I in the presence of PPh₃ in PhMe at 80° for 1 h to give a catalyst solution, which was stored at 80° for 24 h. 3,4-Diacetoxy-1-butene (II) was isomerized in the presence of the stored catalyst solution and AcOH at 130° for 3 h to give a 32:68 mixture of 1,4-diacetoxy-2-butene/II.

IT 403484-12-8P
 RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)
 (storage of transition metal complex catalysts bearing polydentate ligands having P-O bonds by using monodentate phosphines and/or polydentate aryl phosphines as antioxidants)

RN 403484-12-8 CAPLUS

CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-2-naphthalenyl ester (CA INDEX NAME)



L10 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:315029 CAPLUS

DOCUMENT NUMBER: 148:472113

TITLE: Computational descriptors for chelating P,P- and P,N-donor ligands

AUTHOR(S): Fey, Natalie; Harvey, Jeremy N.; Lloyd-Jones, Guy C.; Murray, Paul; Orpen, A. Guy; Osborne, Robert; Purdie, Mark

CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

SOURCE: Organometallics (2008), 27(7), 1372-1383
CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ligand knowledge base approach (LKB) has been extended to capture the properties of 108 bidentate P,P- and P,N-donor ligands (1, L1L2). Several parameters, bite angle for square-planar palladium and tetrahedral zinc chelates $\text{cis}[(\text{L1L2})\text{PdCl}_2]$ (2), $[(\text{L1L2})\text{ZnCl}_2]$ (3), L-M and M-Cl bond lengths (M = Pd, Zn), dissociation free energies for 3, steric requirements evaluated as energy of L1L2-He8-hedge association energy were computed at DFT and MM level for the 108 bidentate ligands L1L2. Frontier orbital energies (EHOMO, ELUMO) and proton affinities (PA) were estimated for ligands 1 by calcn. of these values for truncated monodentate versions. The ligands set 1 is therewith described by a range of DFT-calculated descriptors, capturing ligand properties in a variety of chemical environments. New challenges arising from ligand conformational flexibility and donor asymmetry are discussed, and descriptors are related

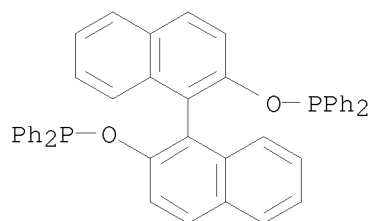
to other parameters, such as the ligand bite angle. A novel map of bidentate ligand space, potentially useful in catalyst design and discovery, has been derived from principal component anal. of the resulting descriptors. In addition, a range of multiple linear regression models were derived for both exptl. and calculated data, considering ligand bite angles in square-planar palladium complexes and ligand dissociation energies from octahedral chromium complexes, resp. These data sets were fitted with models based on LKB descriptors to explore the transferability of descriptors to different coordination environments and to illustrate potential applications of such models in catalyst design, allowing predictions about novel or untested ligands.

IT 179259-59-7 179259-60-0 1018429-17-8
1018429-47-4

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(binding energy, bite angle bond lengths, steric and electronic properties for bidentate diphosphine and phosphine-amine ligands and their metal complexes)

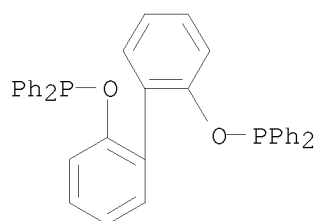
RN 179259-59-7 CAPLUS

CN Phosphinous acid, P,P-diphenyl-, P,P'-[1,1'-binaphthalene]-2,2'-diyl ester (CA INDEX NAME)



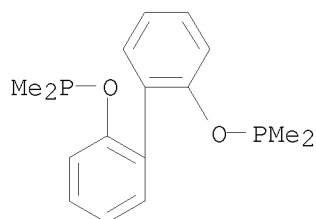
RN 179259-60-0 CAPLUS

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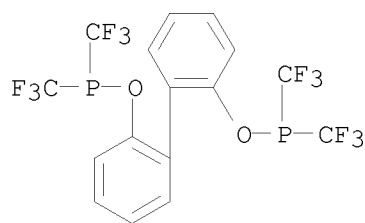


RN 1018429-17-8 CAPLUS

CN Phosphinous acid, P,P-dimethyl-, P,P'-[1,1'-biphenyl]-2,2'-diyl ester (CA INDEX NAME)



RN 1018429-47-4 CAPLUS
 CN Phosphinous acid, P,P-bis(trifluoromethyl)-,
 P,P'-[1,1'-biphenyl]-2,2'-diyl ester (CA INDEX NAME)



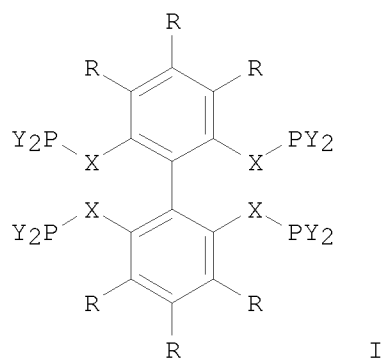
OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
 RECORD (11 CITINGS)
 REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2007:761546 CAPLUS
 DOCUMENT NUMBER: 147:143552
 TITLE: Chelating tetraphosphorus ligands with 1,1'-biphenyl
 backbone for transition metal-catalyzed
 hydroformylation of alkenes and related reactions
 INVENTOR(S): Zhang, Xumu; Yan, Yongjun
 PATENT ASSIGNEE(S): The Penn State Research Foundation, USA
 SOURCE: PCT Int. Appl., 33pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007078859	A2	20070712	WO 2006-US47766	20061215
WO 2007078859	A3	20071129		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
 KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK,
 MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO,
 RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT,
 TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
 CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
 GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
 US 20070203365 A1 20070830 US 2006-639438 20061215
 US 7531698 B2 20090512
 EP 1960409 A2 20080827 EP 2006-845453 20061215
 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
 IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
 BA, HR, MK, RS
 JP 2009519941 T 20090521 JP 2008-545819 20061215
 IN 2008KN02255 A 20090116 IN 2008-KN2255 20080604
 CN 101331144 A 20081224 CN 2006-80047201 20080616
 KR 2008103960 A 20081128 KR 2008-716741 20080710
 US 20090198071 A1 20090806 US 2009-425832 20090417
 PRIORITY APPLN. INFO.: US 2005-750733P P 20051215
 US 2006-639438 A3 20061215
 WO 2006-US47766 W 20061215
 OTHER SOURCE(S): CASREACT 147:143552; MARPAT 147:143552
 GI



AB Tetraphosphines, tetraphosponites, tetraphosphinites,
 tetraphosphorodiamidites and combinations thereof I [R = H, alkyl, aryl,
 alkoxy, aryloxy, CO₂Et, halo, sulfonyl, phosphinyl, amino; Y = alkyl,
 aryl, alkoxy, aryloxy, (un)substituted 1-pyrrolyl; X = O, NH, alkylimino,
 CH₂], useful as ligands for transition metal-catalyzed hydroformylation of
 alkenes, are claimed. Ligands I demonstrate enhanced complexation ability
 at high pressures of CO, thus providing high regioselectivity and n/iso
 ratio of the product aldehydes in the processes, catalyzed by transition
 metal compds., preferably rhodium(I) complexes, at lower ligand/metal
 ratios, compared to monodentate and bidentate ligands. The
 ligands I may be also useful in hydrocarboxylation, hydrocyanation,
 isomerization-formylation, hydroaminomethylation and similar related
 reactions. In an example, ligand I (L1, X = O, R = H, Y = 1-pyrrolyl) was
 prepared by reaction of 4.4 mmol of chlorodi-1-pyrrolylphosphine with 1 mmol
 of 1,1'-biphenyl-2,2',6,6'-tetrol in the presence of 1 mL of Et₃N in 10 mL
 of THF for 6 h at 20°. In subsequent examples, effects of
 hydroformylation reaction conditions and substrate structure were
 explored; hydroformylation of 10 mmol of 1-octene catalyzed by 3:1 mol.

ratio of L1:[Rh(acac)(CO)₂] (1:104 catalyst/substrate ratio) at 100° and 10 atm of CO/H₂ (1:1) for 12 h yielded 1-nonanal with 372:1 n/iso regioselectivity.

IT 920508-98-1P

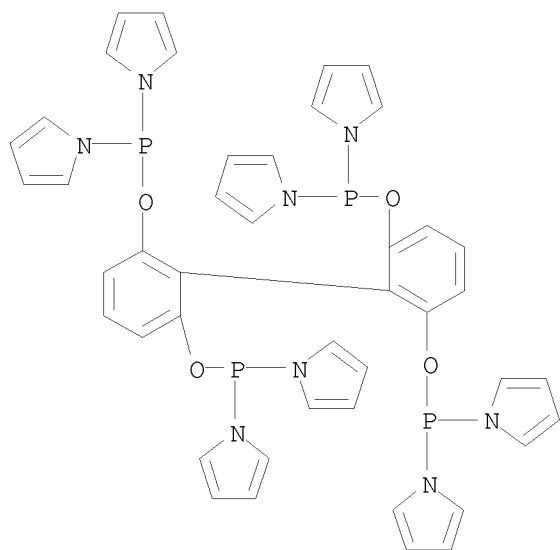
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);

USES (Uses)

(chelating tetraphosphorus ligands with 1,1'-biphenyl backbone as ligands for highly regioselective hydroformylation of alkenes in preparation of linear aldehydes)

RN 920508-98-1 CAPLUS

CN 1H-Pyrrole, 1,1',1'',1''',1'''',1''''',1''''',1''''''-[[1,1'-biphenyl]-2,2',6,6'-tetrayltetrakis(oxyphosphinidyne)]octakis- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L10 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2006:215816 CAPLUS

DOCUMENT NUMBER: 144:450825

TITLE: Total Synthesis of Enantiopure (+)- γ -Lycorane Using Highly Efficient Pd-Catalyzed Asymmetric Allylic Alkylation

AUTHOR(S): Chapsal, Bruno D.; Ojima, Iwao

CORPORATE SOURCE: Department of Chemistry, State University of New York at Stony Brook, Stony Brook, NY, 11794-3400, USA

SOURCE: Organic Letters (2006), 8(7), 1395-1398

CODEN: ORLEF7; ISSN: 1523-7060

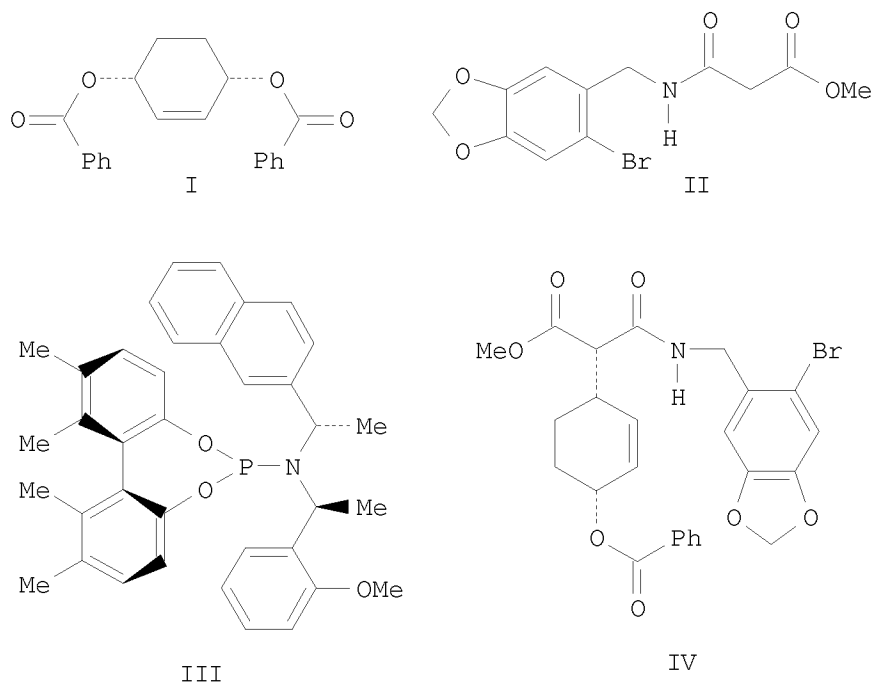
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:450825

GI



AB A highly efficient short total synthesis of (+)- γ -lycorane (>99% ee, 41% overall yield) was achieved by using the asym. allylic alkylation in the key step catalyzed by palladium complexes with novel chiral biphenol-based monodentate phosphoramidite ligands. Thus, reacting dibenzoate I with carbamoylacetate II using [Pd(allyl)Cl]₂ with phosphoramidite ligand III gave alkylated product IV with 99.4% ee in 83% yield. IV was then converted to (+)-lycorane in >99% ee.

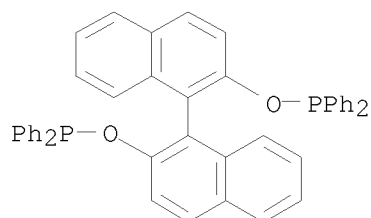
IT 64736-26-1, (S)-BINAPO

RL: CAT (Catalyst use); USES (Uses)

(asym. synthesis of (+)- γ -lycorane via palladium-catalyzed allylic alkylation/desymmetrization)

RN 64736-26-1 CAPLUS

CN Phosphinous acid, P,P-diphenyl-, P,P'-[(1S)-[1,1'-binaphthalene]-2,2'-diyl] ester (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:1329709 CAPLUS
 DOCUMENT NUMBER: 144:71485
 TITLE: Phosphorus-containing catalyst compositions and
 hydroformylation process therewith
 INVENTOR(S): Jeon, You-Moon; Ko, Dong-Hyun; Kwon, O-Hak; Eom,
 Sung-Shik; Lee, Sang-Gi; Moon, Ji-Joong; Park,
 Kwang-Ho
 PATENT ASSIGNEE(S): LG Chem. Ltd., S. Korea
 SOURCE: PCT Int. Appl., 19 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005120705	A1	20051222	WO 2004-KR1646	20040703
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
KR 2005118023	A	20051215	KR 2004-43334	20040612
CN 1863595	A	20061115	CN 2004-80029312	20040703
CN 100431701	C	20081112		
EP 1755782	A1	20070228	EP 2004-774072	20040703
R: DE, FR, GB, SE				
JP 2007507340	T	20070329	JP 2006-532068	20040703
US 20070123735	A1	20070531	US 2006-575147	20060407
PRIORITY APPLN. INFO.:			KR 2004-43334	A 20040612
			WO 2004-KR1646	W 20040703

OTHER SOURCE(S): MARPAT 144:71485

AB Provided are a catalyst composition comprising a bidentate ligand, a monodentate ligand, and a transition metal catalyst and a process of hydroformylation of olefin compds., comprising reacting the olefin compound with a gas mixture of hydrogen and carbon monoxide while being stirred at elevated pressures and temps. in the presence of the catalyst composition to produce an aldehyde. The present catalytic composition demonstrates

the high catalytic activity and option control of selectivity to normal aldehyde or iso aldehyde (N/l selectivity) to a desired value.

IT 247130-61-6

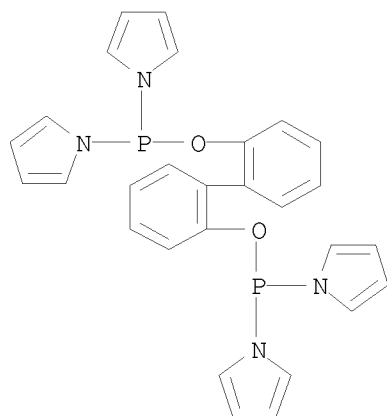
RL: CAT (Catalyst use); USES (Uses)

(phosphorus-containing catalyst compns. and hydroformylation process therewith)

RN 247130-61-6 CAPLUS

CN Phosphinous acid, P,P-di-1H-pyrrol-1-yl-, P,P'-[1,1'-biphenyl]-2,2'-diyl

ester (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:992727 CAPLUS

DOCUMENT NUMBER: 141:425573

TITLE: Process for production of dinitriles by butadiene
hydrocyanation

INVENTOR(S): Bourgeois, Damien; Rosier, Cecile; Leconte, Philippe

PATENT ASSIGNEE(S): Rhodia Polyamide Intermediates, Fr.

SOURCE: Fr. Demande, 18 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2854892	A1	20041119	FR 2003-5673	20030512
FR 2854892	B1	20050624		
WO 2004101498	A2	20041125	WO 2004-FR1110	20040507
WO 2004101498	A3	20050127		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1622863	A2	20060208	EP 2004-742669	20040507

EP 1622863 B1 20080813
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
 CN 1787991 A 20060614 CN 2004-80012864 20040507
 CN 100441566 C 20081210
 JP 2007502854 T 20070215 JP 2006-530334 20040507
 RU 2299194 C2 20070520 RU 2005-138494 20040507
 AT 404530 T 20080815 AT 2004-742669 20040507
 KR 2006040585 A 20060510 KR 2005-721384 20051110
 IN 2005CN02976 A 20070727 IN 2005-CN2976 20051111
 US 20070155979 A1 20070705 US 2006-556628 20060921
 US 7612223 B2 20091103

PRIORITY APPLN. INFO.:

FR 2003-5673 A 20030512
 WO 2004-FR1110 W 20040507

AB The process comprises at least a stage of butadiene hydrocyanation in the presence of a catalytic system containing an organometallic complex having ≥ 1 monodentate organophosphite ligand and ≥ 1 bidentate organophosphorus ligand and optional promoter such as Lewis acid, a stage of distillation to sep. and recover the catalyst. The distillation is done at a molar ratio of organo-P ligand (as P atom) to the number of metal atom of ≤ 15 , or/and at the weight concentration of metal element of $\leq 1.3\%$ and a bottom temperature of $\leq 180^\circ$.

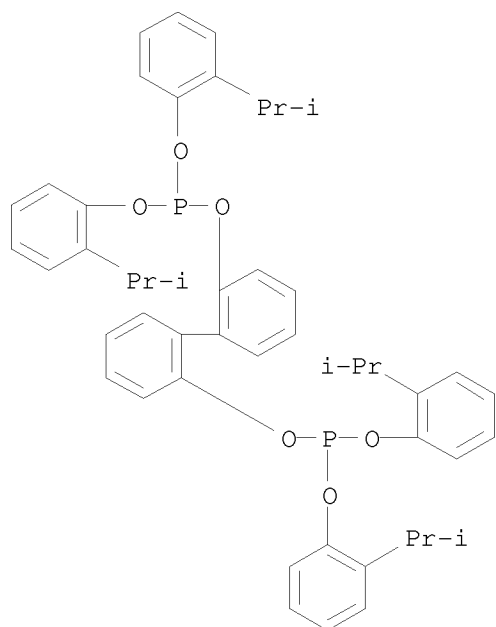
IT 178941-51-0D, metal complex 220472-84-4D, metal complex 330976-81-3D, metal complex 494227-34-8D, metal complex

RL: CAT (Catalyst use); USES (Uses)

(catalyst recovery in process for production of dinitriles by butadiene hydrocyanation)

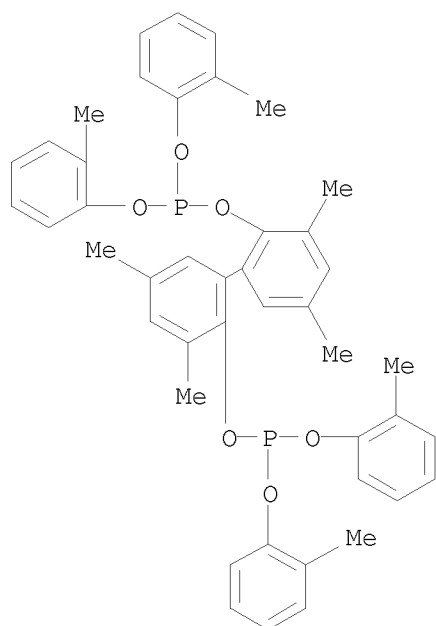
RN 178941-51-0 CAPLUS

CN Phosphorous acid, [1,1'-biphenyl]-2,2'-diyl tetrakis[2-(1-methylethyl)phenyl] ester (9CI) (CA INDEX NAME)



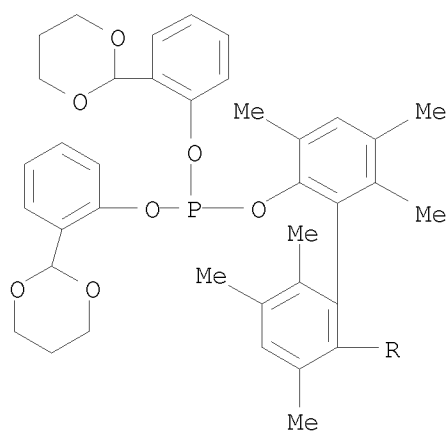
RN 220472-84-4 CAPLUS

CN Phosphorous acid, P,P'-((3,3',5,5'-tetramethyl[1,1'-biphenyl]-2,2'-diyl)
P,P,P',P'-tetrakis(2-methylphenyl) ester (CA INDEX NAME)

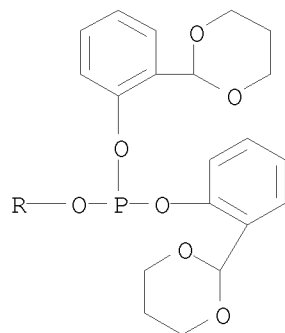


RN 330976-81-3 CAPLUS

CN Phosphorous acid, 3,3',5,5',6,6'-hexamethyl[1,1'-biphenyl]-2,2'-diyl
tetrakis[2-(1,3-dioxan-2-yl)phenyl] ester (9CI) (CA INDEX NAME)

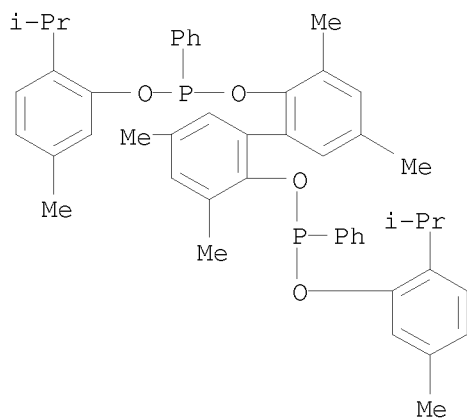


PAGE 1-A



RN 494227-34-8 CAPLUS

CN Phosphonous acid, phenyl-, 3,3',5,5'-tetramethyl[1,1'-biphenyl]-2,2'-diyl bis[5-methyl-2-(1-methylethyl)phenyl] ester (9CI) (CA INDEX NAME)



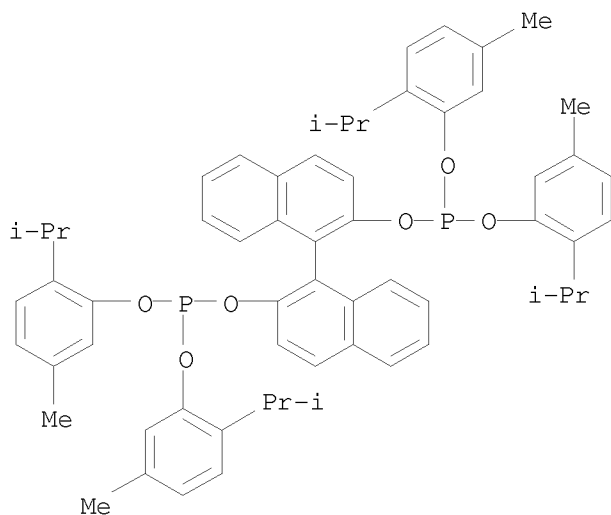
IT 178941-67-8D, metal complex

RL: CAT (Catalyst use); USES (Uses)

(hydrocyanation catalyst; catalyst recovery in process for production of dinitriles by butadiene hydrocyanation)

RN 178941-67-8 CAPLUS

CN Phosphorous acid, [1,1'-binaphthalene]-2,2'-diyl tetrakis[5-methyl-2-(1-methylethyl)phenyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:756724 CAPLUS

DOCUMENT NUMBER: 141:260889

TITLE: Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions

INVENTOR(S): Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York

SOURCE: PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078766	A1	20040916	WO 2003-US5790	20030227
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2003219901	A1	20040928	AU 2003-219901	20030227
WO 2004076464	A2	20040910	WO 2004-US3367	20040227
WO 2004076464	A3	20041216		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

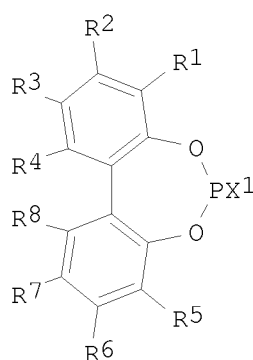
WO 2003-US5790

A 20030227

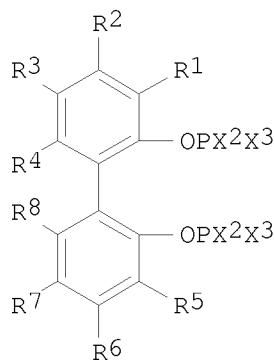
OTHER SOURCE(S):

MARPAT 141:260889

GI



I



II

AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 = (NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic

acid with 70.1% ee; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = OPh, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et₂Zn to 2-cyclohexenone affording (S)-3-methylcyclohexanone with 35% ee.

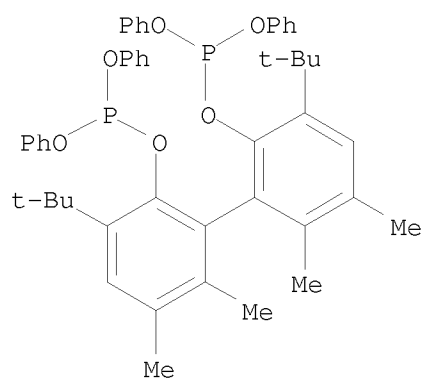
IT 753016-20-5P 753016-21-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(asym. ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

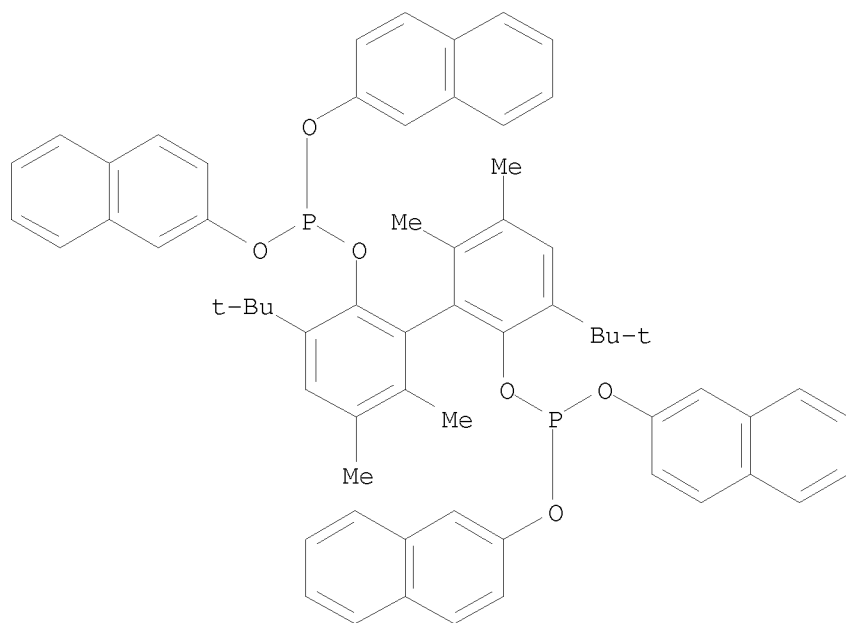
RN 753016-20-5 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetraphenyl ester (9CI) (CA INDEX NAME)



RN 753016-21-6 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



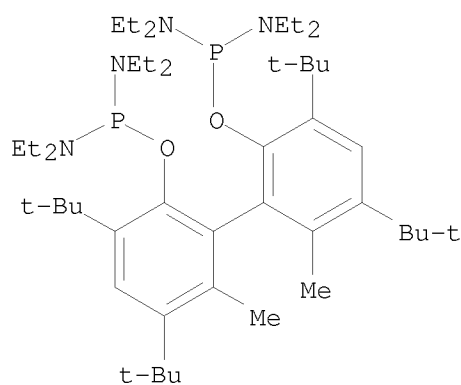
IT 753016-24-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(deamination; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-24-9 CAPLUS

CN Phosphorodiamidous acid, tetraethyl-,
(1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



IT 753016-25-0P, [(S)-3,3',5,5'-Tetra-tert-butyl-6,6'-dimethyl-1,1'-biphenyl-2,2'-diyl] bis(phosphorodichloridite)

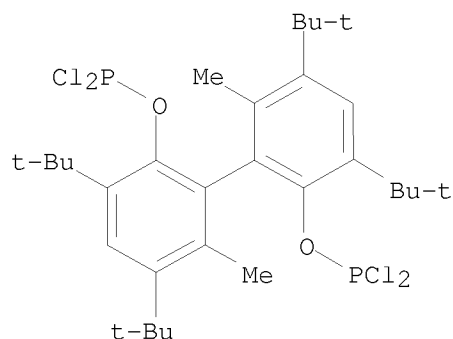
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(esterification; preparation of axially chiral nonracemic mono- and

diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-25-0 CAPLUS

CN Phosphorodichloridous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



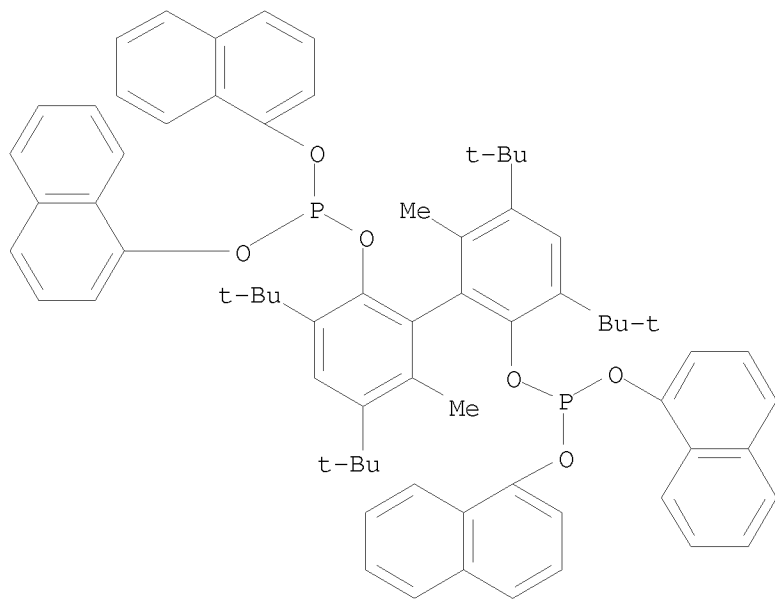
IT 753016-22-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-22-7 CAPLUS

CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-1-naphthalenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:740336 CAPLUS

DOCUMENT NUMBER: 141:243687

TITLE: Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions

INVENTOR(S): Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi; Urata, Hisao

PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

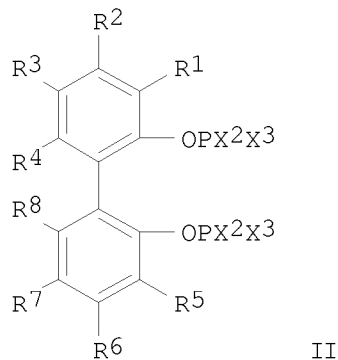
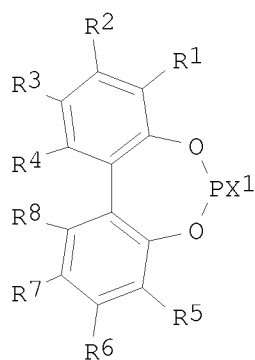
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004076464	A2	20040910	WO 2004-US3367	20040227
WO 2004076464	A3	20041216		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2004078766	A1	20040916	WO 2003-US5790	20030227
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: WO 2003-US5790 A 20030227

OTHER SOURCE(S): MARPAT 141:243687

GI



AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 = (NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic acid with 70.1% ee; (S)-3-methyl-4-oxobutanenitrile was obtained with 96% regioselectivity and 80% ee by asym hydroformylation of 3-butenenitrile; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = N[(R)-CHMePh]2, R1 = R3 = R4 = R5 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et2Zn to 2-cycloheptenone affording (S)-3-methylcycloheptanone with 97.5% ee.

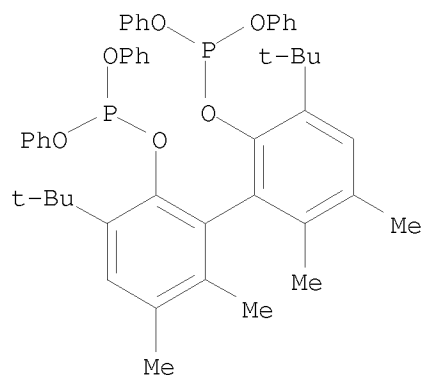
IT 753016-20-5P 753016-21-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(asym. addition ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

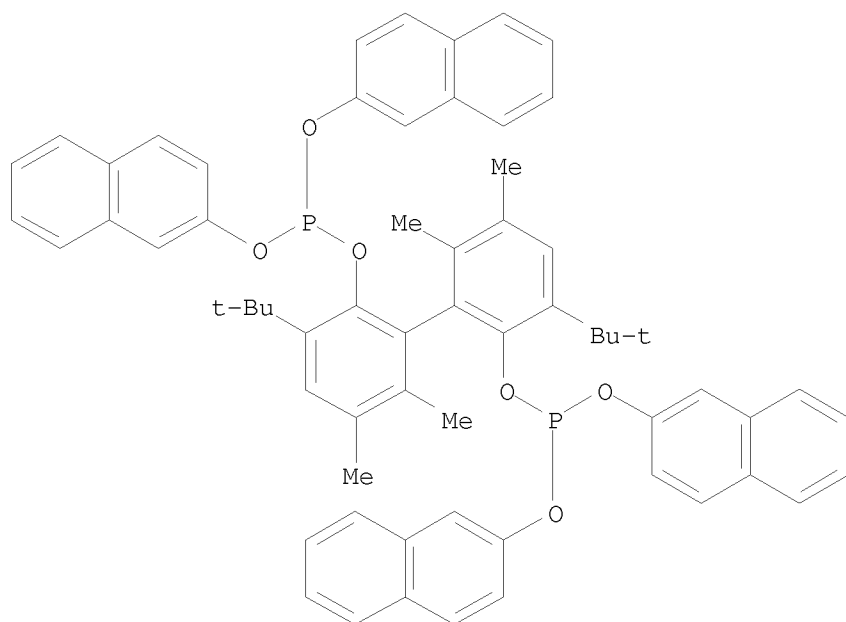
RN 753016-20-5 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetraphenyl ester (9CI) (CA INDEX NAME)



RN 753016-21-6 CAPLUS

CN Phosphorous acid, (1S)-3,3'-bis(1,1-dimethylethyl)-5,5',6,6'-tetramethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

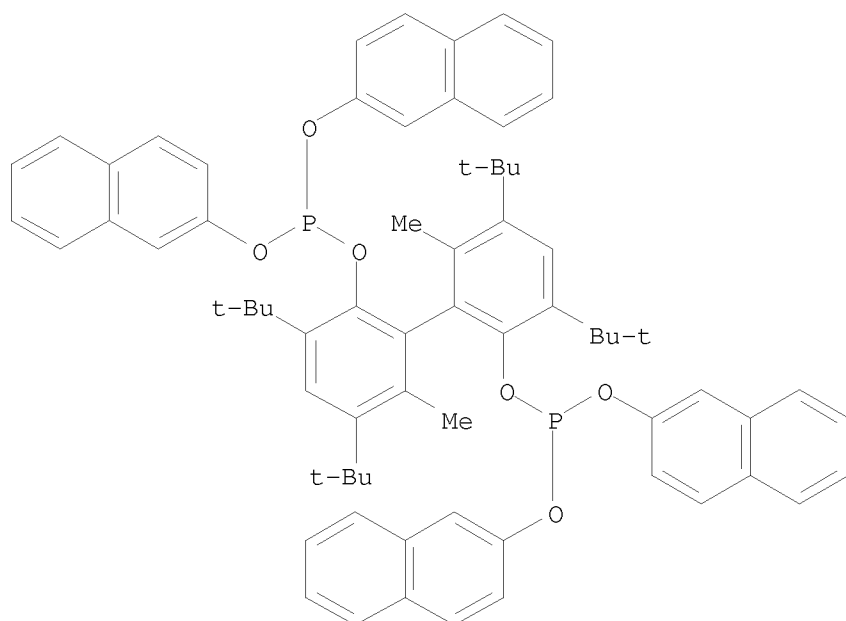


IT 753016-30-7P 753016-35-2P

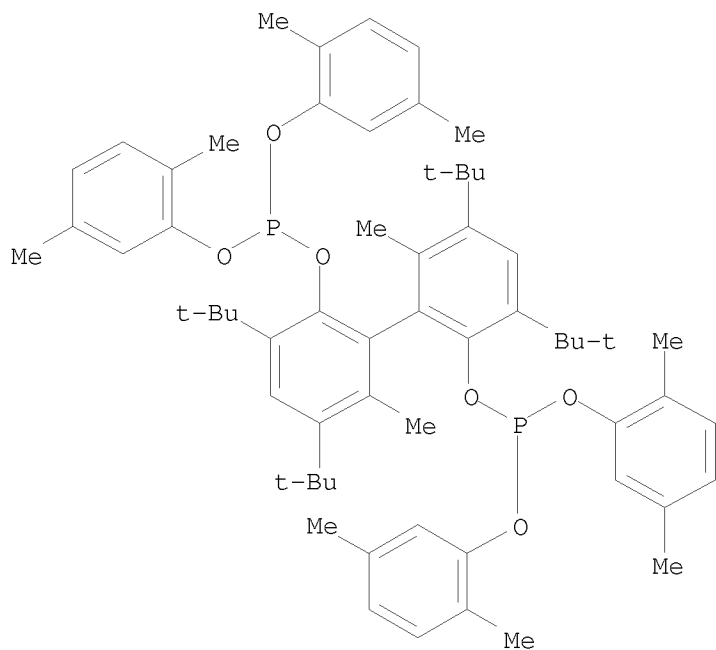
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)

(asym. hydrogenation ligand; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

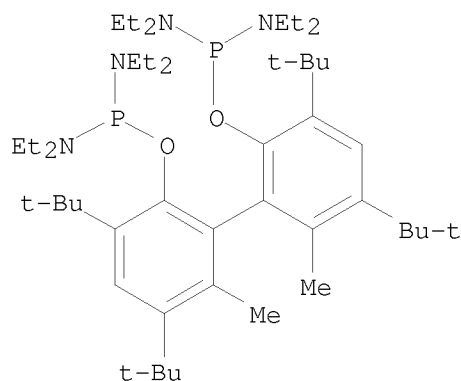
RN 753016-30-7 CAPLUS
 CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-
 dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA
 INDEX NAME)



RN 753016-35-2 CAPLUS
 CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-
 dimethyl[1,1'-biphenyl]-2,2'-diyl tetrakis(2,6-dimethylphenyl) ester (9CI)
 (CA INDEX NAME)



IT 753016-24-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (deamination; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
 RN 753016-24-9 CAPLUS
 CN Phosphorodiamidous acid, tetraethyl-,
 (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)

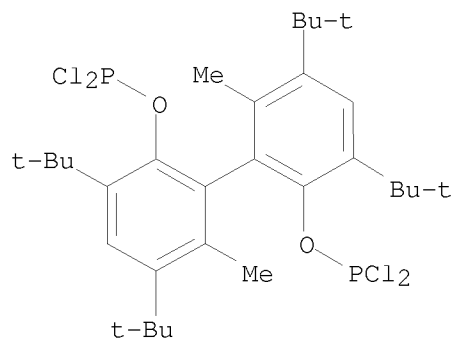


IT 753016-25-0P, [(S)-3,3',5,5'-Tetra-tert-butyl-6,6'-dimethyl-1,1'-biphenyl-2,2'-diyl] bis(phosphorodichloridite)
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(esterification; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-25-0 CAPLUS

CN Phosphorodichloridous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl ester (9CI) (CA INDEX NAME)



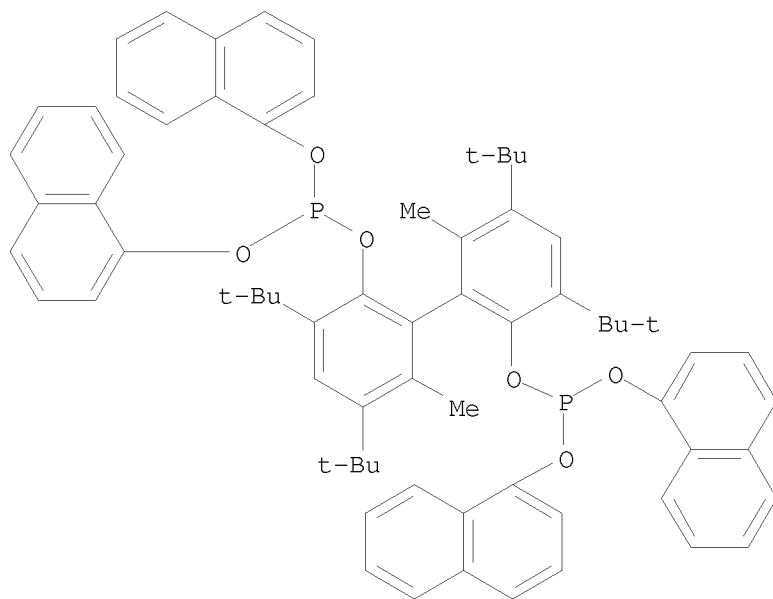
IT 753016-22-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 753016-22-7 CAPLUS

CN Phosphorous acid, (1S)-3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl tetra-1-naphthalenyl ester (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD

(2 CITINGS)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:354301 CAPLUS
 DOCUMENT NUMBER: 140:356943
 TITLE: Preparation of allyl compounds
 INVENTOR(S): Tanaka, Yoshiyuki; Takai, Masaki
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 56 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004131491	A	20040430	JP 2003-315716	20030908
US 20040147757	A1	20040729	US 2003-648210	20030827
US 7119222	B2	20061010		
US 20050075518	A1	20050407	US 2003-650697	20030829
US 7173157	B2	20070206		
US 20060106181	A1	20060518	US 2005-300290	20051215
US 7241857	B2	20070710		
PRIORITY APPLN. INFO.:			JP 2002-261870	A 20020906
			JP 2002-252900	A 20020830
			JP 2002-252901	A 20020830
			JP 2002-260452	A 20020905
			US 2003-648210	A3 20030827

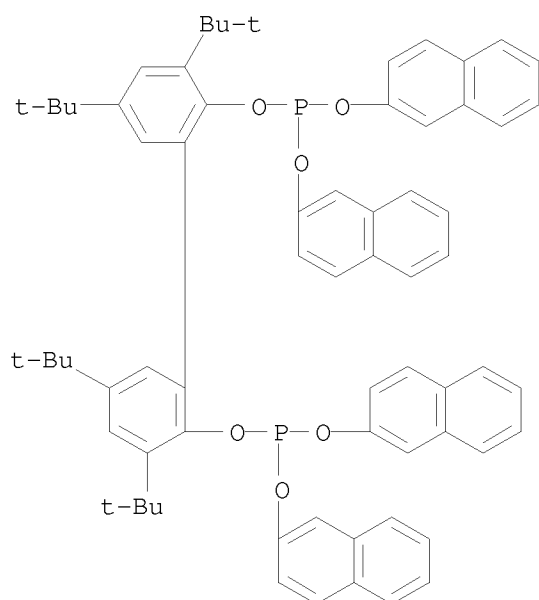
OTHER SOURCE(S): MARPAT 140:356943

AB Allyl compds. are prepared by reaction of allyl compound reactants with nucleophiles by using catalysts containing transition metal compds. having ≥ 1 Group 8-10 transition metals and monodentate ligands P(OR1)(OR2)(OR3) [R1-R3 = (un)substituted alkyl] in the presence of ammonium compds. in the reaction system. Multidentate ligands of phosphites can be also used as catalysts. AcOH was treated with 3,4-diacetoxy-1-butene in the presence of 4-methoxypyridine and a catalyst prepared from trisdibenzylideneacetonedipalladium and tetra(1-naphthyl) 3,3',-5,5'-tetra-(tert-butyl)-6,6'-dimethyl-1'1'-biphenyl-2'2'-diyl diphosphite at 120° to give 1,4-diacetoxy-2-butene [198979-98-5] with reaction rate constant 0.88 h⁻¹.

IT 198979-95-2 198979-98-5 403484-12-8
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst ligand; preparation of allyl compds. by reaction of allyl compound reactants with nucleophiles in the presence of ammonium compds. and transition metal catalysts)

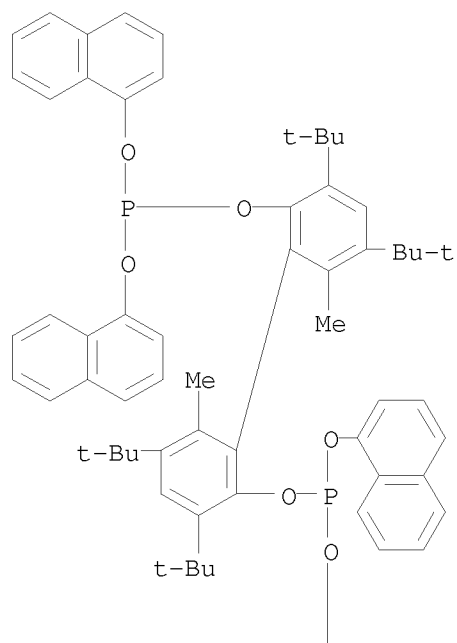
RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

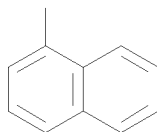


RN 198979-98-5 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-1-naphthalenyl ester (CA INDEX NAME)

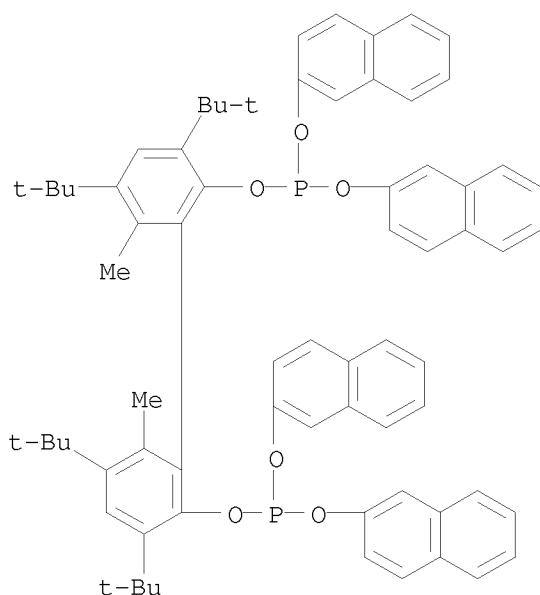
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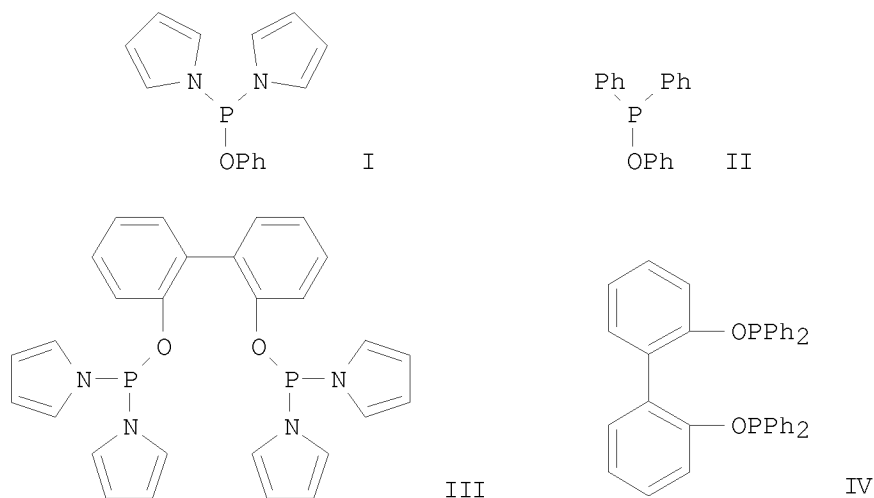
RN 403484-12-8 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-2-naphthalenyl ester
 (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
 (1 CITINGS)

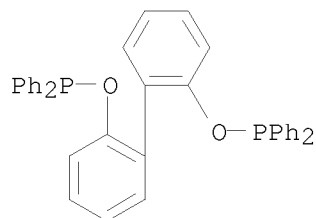
L10 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2002:627995 CAPLUS
 DOCUMENT NUMBER: 137:319550
 TITLE: Rhodium-Catalyzed Hydroformylation and
 Deuterioformylation with Pyrrolyl-Based Phosphorus
 Amidite Ligands: Influence of Electronic Ligand
 Properties
 AUTHOR(S): van der Slot, Saskia C.; Duran, Josep; Luten, Jordy;
 Kamer, Paul C. J.; van Leeuwen, Piet W. N. M.
 CORPORATE SOURCE: Institute of Molecular Chemistry, University of
 Amsterdam, Amsterdam, 1018 WV, Neth.
 SOURCE: Organometallics (2002), 21(19), 3873-3883
 CODEN: ORGND7; ISSN: 0276-7333
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:319550
 GI

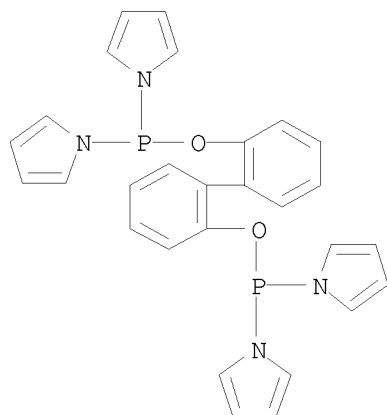


AB The influence of electronic ligand properties on the catalyst performance in the rhodium-catalyzed hydroformylation of alkenes was investigated. Two bidentate phosphorus amidite and phosphinite ligands were synthesized: 1,1'-biphenyl-2,2'-diyl-bis(dipyrrolylphosphoramidite) (III) and 1,1'-biphenyl-2,2'-diylbis(diphenylphosphinite) (IV). Their monodentate analogs also were studied: phenyldipyrrolylphosphoramidite (I) and Ph diphenylphosphinite (II). These two sets of ligands have very similar steric properties but the amidites are much stronger π -acceptor ligands. Spectroscopic studies showed that under hydroformylation reaction conditions the monodentate ligands I and II form mixts. of $\text{HRhL}_2(\text{CO})_2$ and $\text{HRhL}_3(\text{CO})$ complexes depending on the ligand and rhodium concns. and the carbon monoxide pressure. Depending on the reaction conditions, the bidentate ligands III and IV form mixts. of $\text{HRh}(\text{L-L})(\text{CO})_2$ and $\text{HRh}(\text{L-L})(\text{L-L}')(\text{CO})$, where L-L' functions as a monodentate. All ligands were tested in the hydroformylation reaction of oct-1-ene. A high π -acidity of the ligand resulted in a high rate of hydroformylation. The monodentate ligands I and II showed moderate selectivity for the linear aldehyde. The catalyst formed with the bidentate phosphorus amidite ligand III revealed high regioselectivity for the linear aldehyde (ratio 1/b .simeq.100) at a high rate together with a moderate selectivity for isomerization (.apprx.7%). Deuterioformylation expts. of 1-hexene showed that the hydride (deuteride) migration is reversible in the hydroformylation system formed by III. Surprisingly, both the linear rhodium-alkyl and the branched rhodium-alkyl complex undergo β -hydride elimination. Also, the 2-hexylrhodium intermediate regenerates more often monodeuterated 1-hexene than 2-hexene. The rhodium hydride species formed this way reacts relatively slowly with the excess of D₂ and as a result large amts. of monodeuterated heptanal (40% D₁ vs. 60% D₂) and monodeuterated 1-hexene are formed. At higher conversions the

latter gives trisdeuterated heptanal as well as bisdeuterated heptanal.
 IT 179259-60-0P 247130-61-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and complexation with rhodium to give hydroformylation
 catalysts)
 RN 179259-60-0 CAPLUS
 CN Phosphinous acid, P,P-diphenyl-, P,P'-[1,1'-biphenyl]-2,2'-diyl ester (CA
 INDEX NAME)

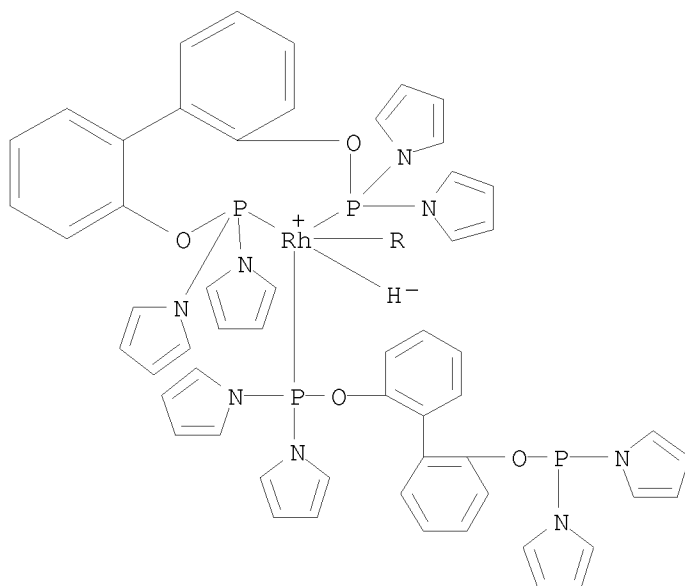


RN 247130-61-6 CAPLUS
 CN Phosphinous acid, P,P-di-1H-pyrrol-1-yl-, P,P'-[1,1'-biphenyl]-2,2'-diyl
 ester (CA INDEX NAME)

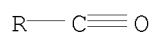


IT 471273-69-5P 471273-71-9P 471273-81-1P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
 USES (Uses)
 (preparation of rhodium hydrido dipyrrolylphosphorodiamidite and
 diphenylphosphinite complexes and catalytic activity for regioselective
 hydroformylation of alkenes)
 RN 471273-69-5 CAPLUS
 CN Rhodium, [[1,1'-biphenyl]-2,2'-diyl
 bis(di-1H-pyrrol-1-ylphosphinite-κP)]carbonyl[2'-[(di-1H-pyrrol-1-
 ylphosphino)oxy][1,1'-biphenyl]-2-yl
 di-1H-pyrrol-1-ylphosphinite-κP]hydro-, (TB-5-34)- (9CI) (CA INDEX
 NAME)

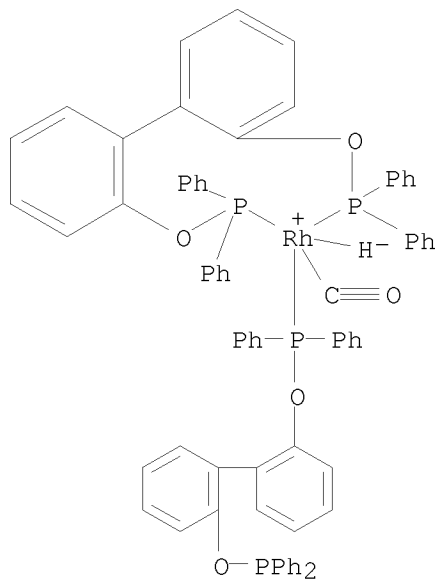
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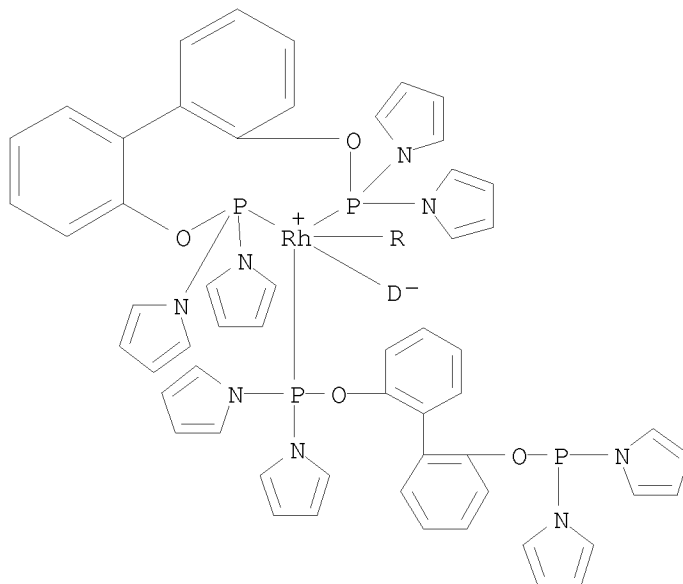


RN 471273-71-9 CAPLUS
 CN Rhodium, [[1,1'-biphenyl]-2,2'-diyl
 bis(diphenylphosphinite-κP)]carbonyl[2'-
 [(diphenylphosphino)oxy][1,1'-biphenyl]-2-yl
 diphenylphosphinite-κP]hydro-, (TB-5-34)- (9CI) (CA INDEX NAME)

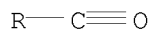


RN 471273-81-1 CAPLUS
 CN Rhodium, [[1,1'-biphenyl]-2,2'-diyl
 bis(di-1H-pyrrol-1-ylphosphinite-κP)]carbonyl[2'-[(di-1H-pyrrol-1-
 ylphosphino)oxy][1,1'-biphenyl]-2-yl
 di-1H-pyrrol-1-ylphosphinite-κP]hydro-d-, (TB-5-34)- (9CI) (CA
 INDEX NAME)

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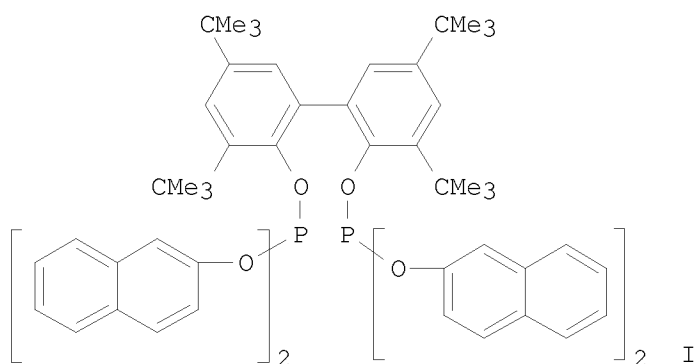
PAGE 2-A



OS.CITING REF COUNT: 36 THERE ARE 36 CAPLUS RECORDS THAT CITE THIS
 RECORD (37 CITINGS)
 REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1999:596871 CAPLUS
 DOCUMENT NUMBER: 131:228491
 TITLE: Method of preparation of aldehyde by selective
 hydroformylation of olefin in presence of monovalent
 phosphite compound
 INVENTOR(S): Wada, Yasuhiro; Tanaka, Yoshiyuki; Urata, Takao
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11255696	A	19990921	JP 1998-56503	19980309
JP 3903575	B2	20070411		
PRIORITY APPLN. INFO.:			JP 1998-56503	19980309
OTHER SOURCE(S):			CASREACT 131:228491; MARPAT 131:228491	
GI				



AB In preparation of an aldehyde by hydroformylation of olefin with carbon monoxide and hydrogen in the presence of a group VIII metal and an organic polydentate phosphite, the reaction is carried out in the presence of a monodentate phosphite represented by formula $\text{Ar}_3\text{-P}(\text{OAr}_1)\text{OAr}_2$ [Ar_1 - Ar_3 = (un)substituted aromatic organic group, provided that at least two of Ar_1 - Ar_3 possess a branched hydrocarbonyl group at one of the two positions ortho to the phosphite oxygen atom and hydrogen at the other position] in the reaction system. The copresence of the monodentate phosphite ligand improves the catalyst activity and selectivity in a continuous operation and suppresses the side reaction, i.e. reduction of olefins, and can stably provide straight-chain aldehydes which are industrially useful. Thus, 55 mL PhMe, 5 mL heptane, 19.7 mg $[\text{Rh}(\text{OAc})(\text{COD})]_2$ (COD = 1,5-cyclooctadiene), divalent phosphite (I) 2.0 mol/1 g atom Rh, and tris[3,6,8-tri(tert-butyl)-2-naphthyl] phosphite (monovalent phosphite) 4.0 mol/1 g atom Rh were charged in an autoclave. After closing the autoclave and thoroughly purging the inside of the autoclave with N₂, 4.50 g propylene was introduced under pressure followed by introducing water gas (CO/H₂) to a total pressure of 10.0 atm, and the reaction mixture was allowed to react for 1.03-2.60 h while keeping the pressure constant by feeding water gas through a automated pressure regulator to give n-butanal with 97.6% selectivity.

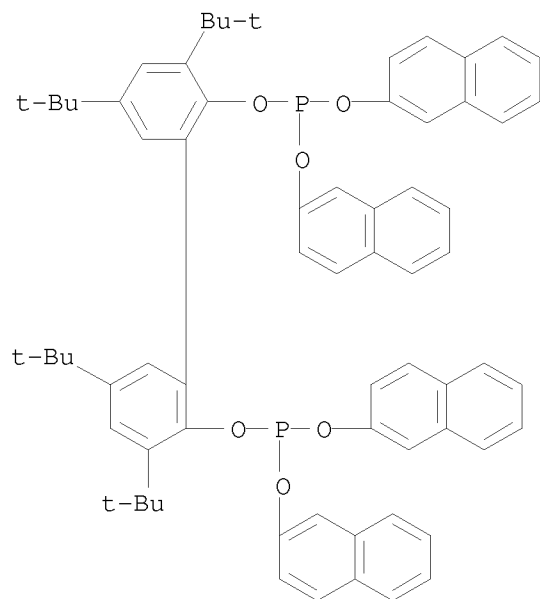
IT 198979-95-2 198979-98-5

RL: CAT (Catalyst use); USES (Uses)

(preparation of aldehyde by selective hydroformylation of olefin with carbon monoxide and hydrogen in presence of group VIII metal-bidentate phosphite complex and monodentate phosphite)

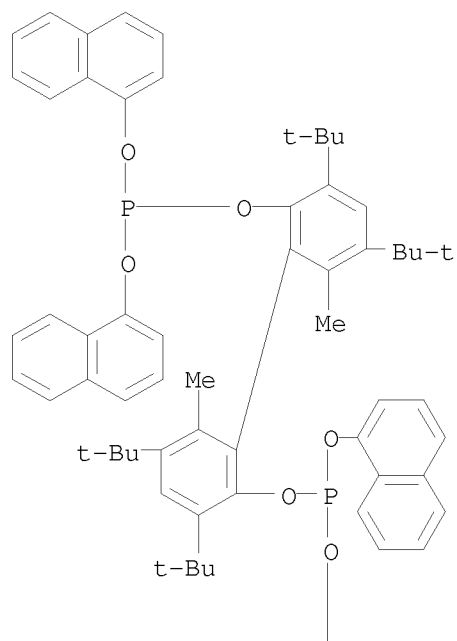
RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)

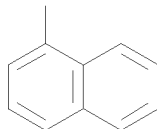


RN 198979-98-5 CAPLUS
 CN Phosphorous acid, P,P'-[3,3',5,5'-tetrakis(1,1-dimethylethyl)-6,6'-dimethyl[1,1'-biphenyl]-2,2'-diyl] P,P,P',P'-tetra-1-naphthalenyl ester (CA INDEX NAME)

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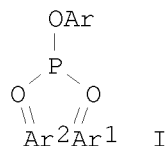
PAGE 2-A



L10 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1999:583153 CAPLUS
 DOCUMENT NUMBER: 131:199415
 TITLE: Preparation of aldehydes
 INVENTOR(S): Wada, Yasuhiro; Tanaka, Yoshiyuki; Urata, Takao
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11246464	A	19990914	JP 1998-52999	19980305
PRIORITY APPLN. INFO.:			JP 1998-52999	19980305
OTHER SOURCE(S):	MARPAT	131:199415		

GI



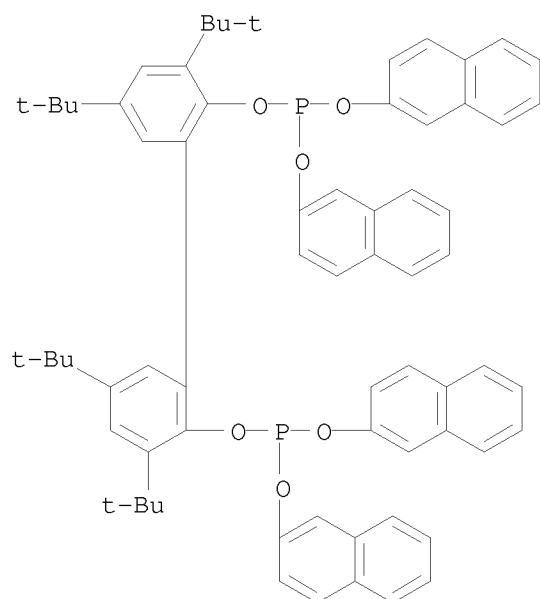
AB Title compds. are prepared by hydroformylation of olefins with CO and H in the presence of cyclic monodentate phosphites I (Ar1, Ar2 = ≥ 1 branched hydrocarbyl-substituted divalent aromatic organic group; Ar = aromatic organic group having no bulky group at o-position to OP) and catalysts containing Group VIII metals and organic multidentate phosphites. Propylene was reacted with a H₂/CO gaseous mixture in the presence of Rh[(OAc)(COD)]₂, Q1[OPQ22]₂ (Q1 = 2,4-tert-butyl-1,6-phenylene-3,5-tert-butyl-1,6-phenylene, Q2 = 2-naphthyl), and I (Ar1Ar2 = same as Q1, Ar = 2-naphthyl) in PhMe at 70° under 10.0 atm for 0.85-1.10 h to give n-aldehyde with 97.9% selectivity.

IT 198979-95-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalyst ligand; preparation of aldehydes by hydroformylation of olefins)

with Group VIII metal-multidentate phosphite catalysts and cyclic monodentate phosphites)

RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



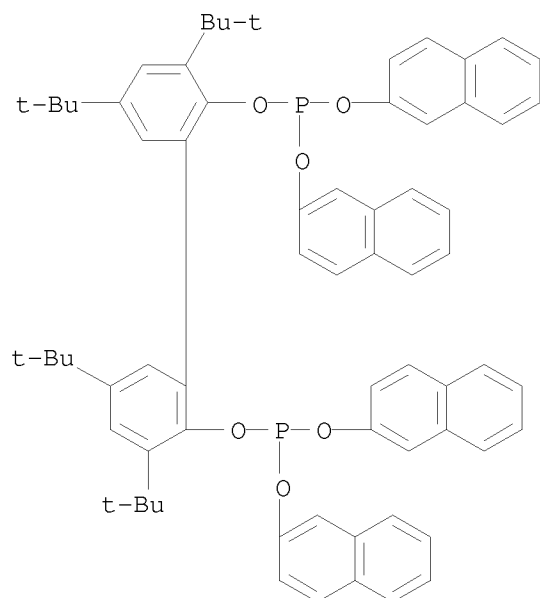
IT 198979-95-2D, complex with Rh

RL: CAT (Catalyst use); USES (Uses)

(preparation of aldehydes by hydroformylation of olefins with Group VIII metal-multidentate phosphite catalysts and cyclic monodentate phosphites)

RN 198979-95-2 CAPLUS

CN Phosphorous acid, 3,3',5,5'-tetrakis(1,1-dimethylethyl)[1,1'-biphenyl]-2,2'-diyl tetra-2-naphthalenyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:300852 CAPLUS

DOCUMENT NUMBER: 128:323141

ORIGINAL REFERENCE NO.: 128:64031a,64034a

TITLE: Process for preparation of an aldehyde by hydroformylation of an unsaturated organic compound

INVENTOR(S): Borman, Peter Cornelis; Gelling, Onko Jan

PATENT ASSIGNEE(S): DSM N.V., Neth.

SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 839787	A1	19980506	EP 1996-203070	19961104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2270521	A1	19980514	CA 1997-2270521	19971030
WO 9819984	A1	19980514	WO 1997-NL595	19971030
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9858830	A	19980529	AU 1998-58830	19971030
EP 937023	A1	19990825	EP 1997-954493	19971030
EP 937023	B1	20011004		

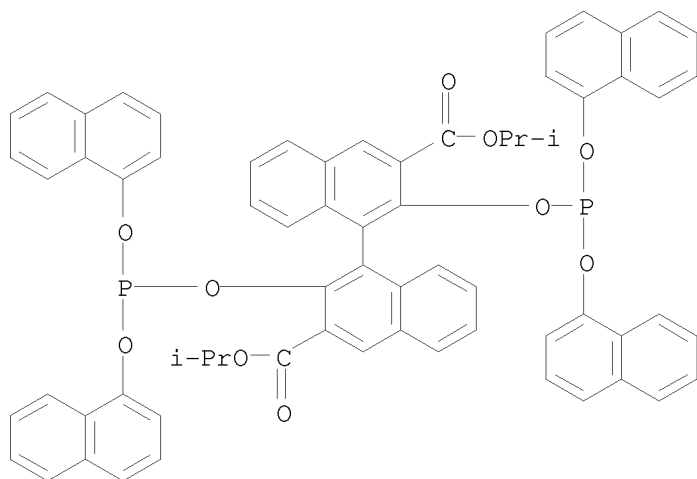
EP 937023	B2	20060208		
R: BE, DE, ES, FR, GB, IT, NL				
CN 1241993	A	20000119	CN 1997-181069	19971030
CN 1117723	C	20030813		
JP 2001504099	T	20010327	JP 1998-521246	19971030
ES 2165102	T3	20020301	ES 1997-954493	19971030
US 6153800	A	20001128	US 1999-303680	19990503
KR 2000053058	A	20000825	KR 1999-703967	19990504
HK 1024465	A1	20040507	HK 2000-103790	20000622
PRIORITY APPLN. INFO.:			EP 1996-203070	A 19961104
			US 1996-32672P	P 19961209
			WO 1997-NL595	W 19971030

OTHER SOURCE(S): MARPAT 128:323141

AB The process uses a catalyst system comprising rhodium or iridium, a multidentate organic phosphite ligand, and a monodentate phosphine. The process can advantageously be carried out for the preparation of Me 5-formylvalerate, which is an intermediate in the preparation of ϵ -caprolactam or adipic acid, which are in turn raw materials for the preparation of nylon 6 and nylon 66, resp.

IT 196299-56-6
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts for preparation of aldehydes by hydroformylation of unsatd. organic compds.)

RN 196299-56-6 CAPLUS
 CN [1,1'-Binaphthalene]-3,3'-dicarboxylic acid, 2,2'-bis[[bis(1-naphthalenyloxy)phosphino]oxy]-, 3,3'-bis(1-methylethyl) ester (CA INDEX NAME)



OS.CITING REF COUNT:	4	THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT:	4	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST	ENTRY 76.56	SESSION 502.54
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-10.66	-18.04

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:38:01 ON 18 NOV 2009